

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
 Data File : BM047320.D
 Acq On : 22 Aug 2024 17:10
 Operator : RC/JU
 Sample : P3671-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S-911-KI-SO-0-0.5-081924

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047320.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.258	60	63	84	rVB	150551	269337	3.06%	0.321%
2	4.563	280	285	301	rVB	196903	298712	3.39%	0.356%
3	5.010	355	361	380	rBV	2922613	4364821	49.51%	5.196%
4	6.569	619	626	639	rBV	2902321	4694406	53.25%	5.589%
5	7.351	752	759	770	rBV	1105122	1728749	19.61%	2.058%
6	7.651	804	810	819	rVB	1290029	1950685	22.13%	2.322%
7	8.210	900	905	911	rVB	138432	210529	2.39%	0.251%
8	8.463	941	948	949	rBV	117407	171424	1.94%	0.204%
9	8.498	949	954	975	rVB	1940982	3190457	36.19%	3.798%
10	9.081	1049	1053	1060	rVB	66749	105297	1.19%	0.125%
11	9.769	1165	1170	1175	rBV	71265	125618	1.43%	0.150%
12	10.104	1220	1227	1244	rVB	1416473	2370579	26.89%	2.822%
13	10.869	1351	1357	1361	rBV	128833	252087	2.86%	0.300%
14	12.616	1647	1654	1669	rBV	4274114	6644945	75.38%	7.911%
15	13.322	1770	1774	1780	rVB2	62933	94437	1.07%	0.112%
16	13.863	1860	1866	1870	rBV	81610	117282	1.33%	0.140%
17	14.010	1884	1891	1900	rBV	2095515	3181898	36.10%	3.788%
18	14.092	1900	1905	1909	rVB3	56271	101256	1.15%	0.121%
19	14.269	1926	1935	1941	rBV2	365475	645796	7.33%	0.769%
20	14.345	1944	1948	1953	rVB	109414	152726	1.73%	0.182%
21	14.492	1969	1973	1979	rVB5	49883	88980	1.01%	0.106%
22	15.222	2093	2097	2103	rVB4	59217	103882	1.18%	0.124%
23	15.404	2121	2128	2129	rBV4	72845	119396	1.35%	0.142%
24	15.480	2137	2141	2143	rBV	101545	141893	1.61%	0.169%
25	15.521	2143	2148	2159	rVV	3780252	5718120	64.87%	6.807%
26	15.604	2159	2162	2173	rVB2	115962	230571	2.62%	0.274%
27	15.763	2184	2189	2193	rBV	481607	644628	7.31%	0.767%
28	16.004	2226	2230	2234	rBV3	61054	89909	1.02%	0.107%
29	16.221	2261	2267	2274	rBV6	62807	135944	1.54%	0.162%
30	16.345	2283	2288	2295	rBV2	181911	384097	4.36%	0.457%
31	16.439	2299	2304	2311	rVV	239915	344725	3.91%	0.410%
32	16.774	2348	2361	2371	rBV	2683697	4566078	51.80%	5.436%
33	16.898	2378	2382	2390	rVB3	113221	196560	2.23%	0.234%
34	16.986	2391	2397	2401	rBV2	441130	826068	9.37%	0.983%
35	17.068	2408	2411	2420	rVB5	148003	257997	2.93%	0.307%
36	17.539	2478	2491	2507	rBV2	744288	2030632	23.04%	2.417%

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Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M

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37	17.680	2508	2515	2518	rBV	1003147	1501838	17.04%	1.788%
38	17.715	2518	2521	2526	rVB	887135	1122562	12.73%	1.336%
39	17.821	2535	2539	2549	rVB2	304497	490051	5.56%	0.583%
40	18.639	2674	2678	2687	rVV2	273793	427384	4.85%	0.509%
41	18.857	2710	2715	2719	rBV	165396	255104	2.89%	0.304%
42	19.015	2737	2742	2752	rBV	361086	533544	6.05%	0.635%
43	19.221	2773	2777	2782	rBV	104085	133633	1.52%	0.159%
44	19.368	2798	2802	2806	rBV	355930	495158	5.62%	0.589%
45	19.409	2806	2809	2810	rVV	351449	368557	4.18%	0.439%
46	19.445	2810	2815	2827	rVB	6999536	8815217	100.00%	10.494%
47	19.592	2835	2840	2846	rVB	511684	606155	6.88%	0.722%
48	19.757	2864	2868	2870	rBV	164713	211461	2.40%	0.252%
49	19.833	2877	2881	2886	rBV	241816	306873	3.48%	0.365%
50	19.892	2886	2891	2900	rVB2	354164	545709	6.19%	0.650%
51	20.109	2925	2928	2932	rBV3	100258	123914	1.41%	0.148%
52	20.751	3032	3037	3048	rBV	1954080	2913153	33.05%	3.468%
53	21.015	3077	3082	3087	rBV	2609485	3458662	39.24%	4.117%
54	21.074	3089	3092	3100	rVB2	239455	332507	3.77%	0.396%
55	21.227	3115	3118	3128	rVB3	151814	269206	3.05%	0.320%
56	21.439	3150	3154	3164	rVB3	167836	310339	3.52%	0.369%
57	21.762	3199	3209	3221	rBV	2199006	5056032	57.36%	6.019%
58	22.150	3271	3275	3283	rVB2	231505	391813	4.44%	0.466%
59	22.974	3410	3415	3420	rBV	631541	1115225	12.65%	1.328%
60	23.039	3420	3426	3439	rVB2	661509	1693468	19.21%	2.016%
61	23.709	3532	3540	3553	rVB	1331472	3265222	37.04%	3.887%
62	24.656	3695	3701	3710	rVB	349639	824710	9.36%	0.982%
63	24.774	3714	3721	3737	rVB	542755	1881964	21.35%	2.240%

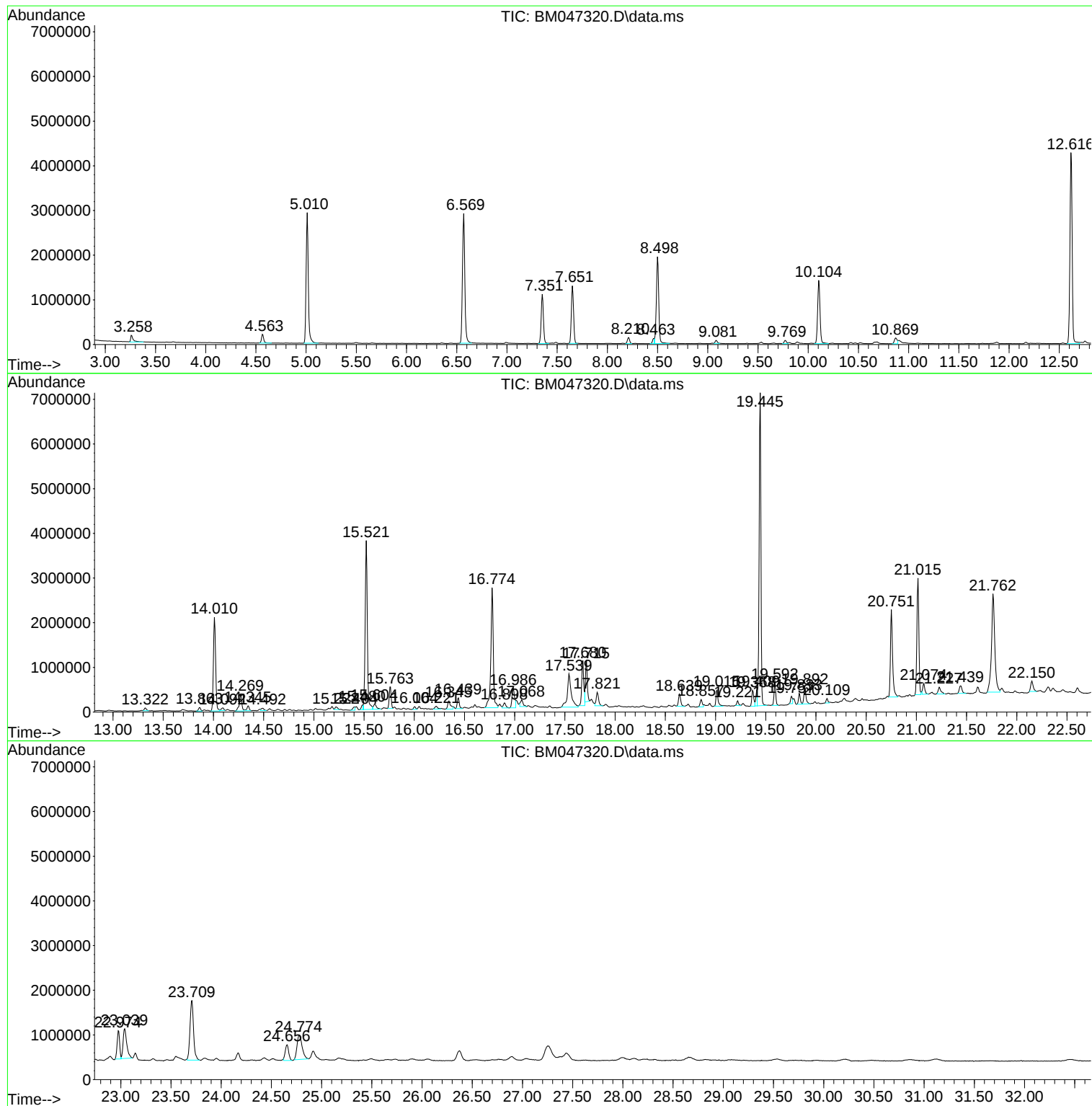
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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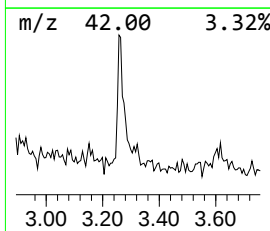
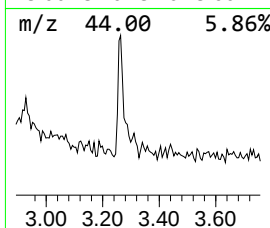
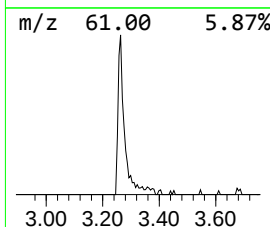
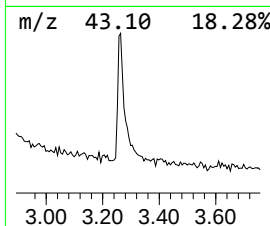
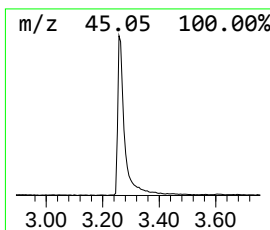
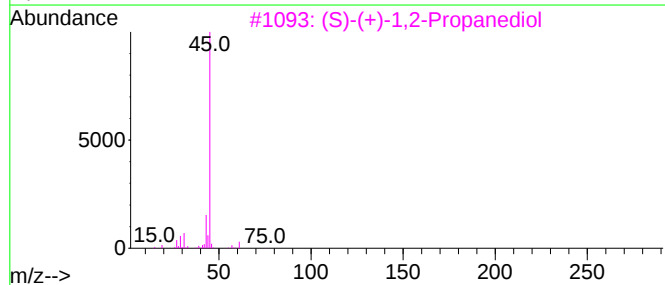
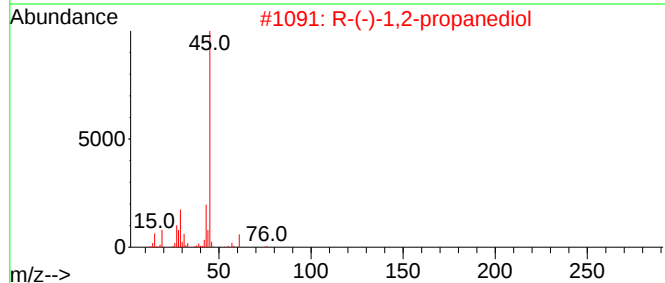
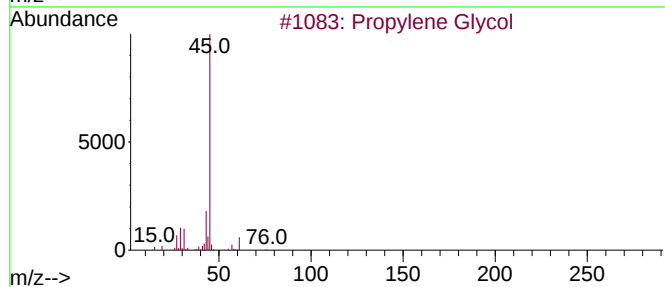
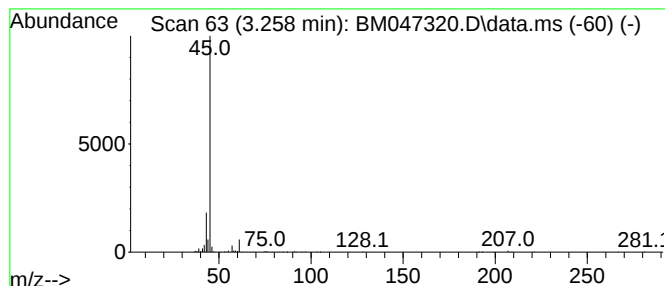
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propylene Glycol Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.258	3.12 ng	269337	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	78
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			2-Butanol	74	C4H10O	000078-92-2	39



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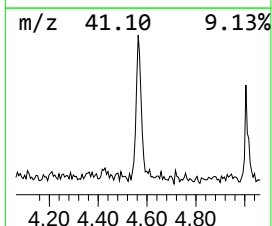
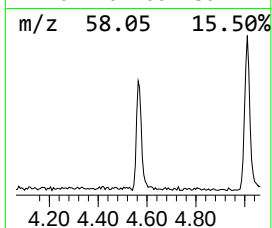
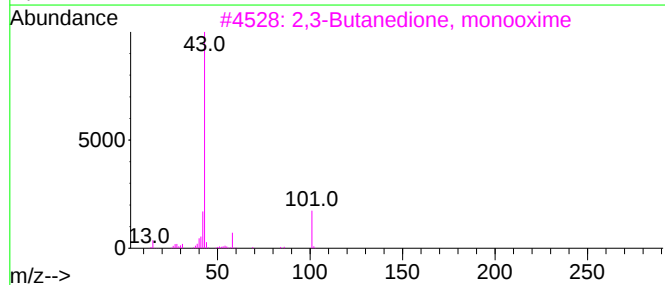
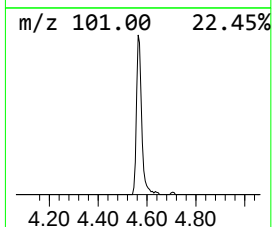
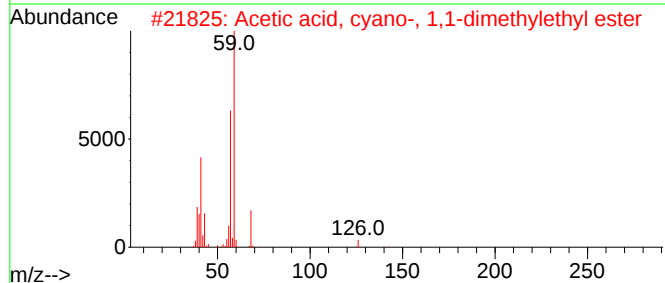
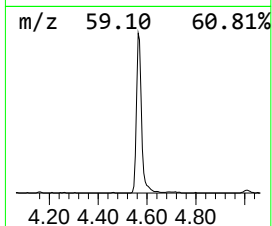
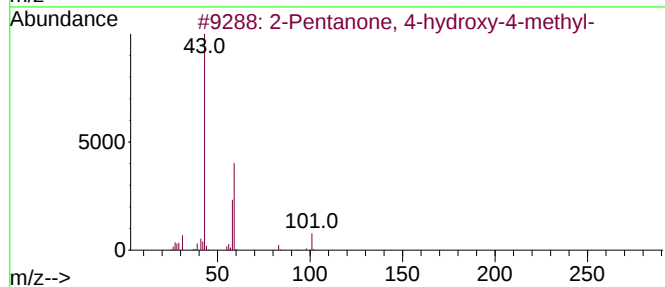
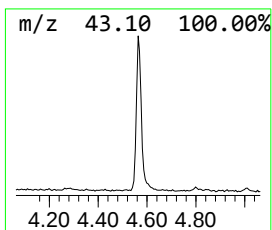
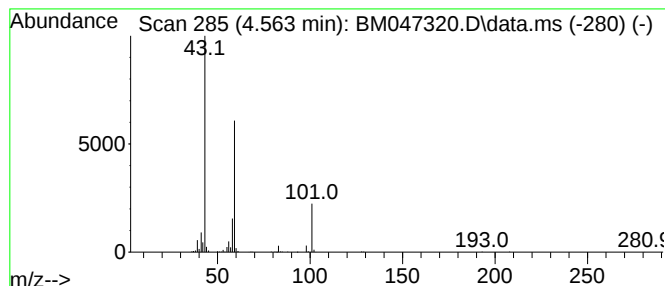
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	3.46 ng	298712	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Butane	58	C4H10	000106-97-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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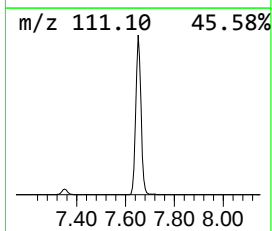
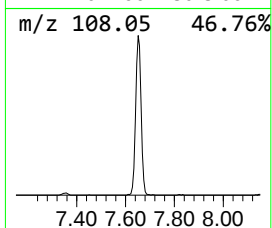
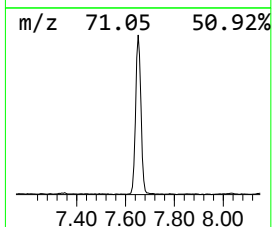
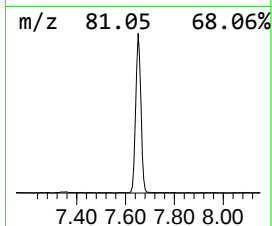
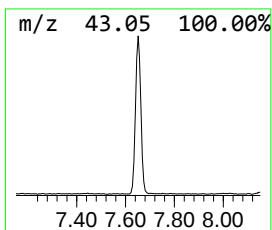
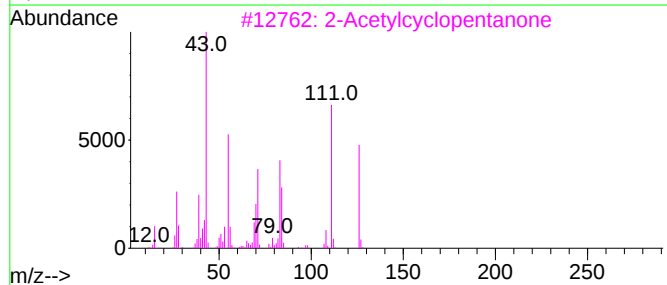
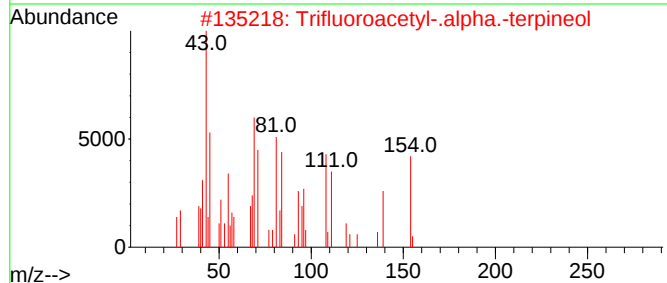
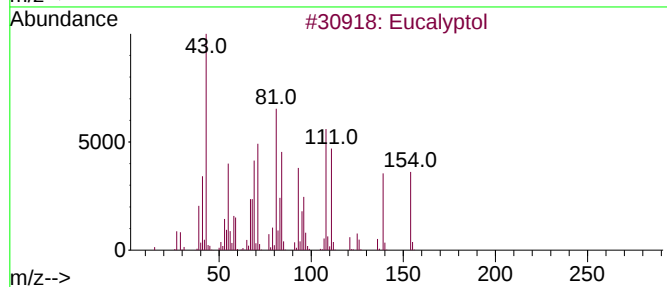
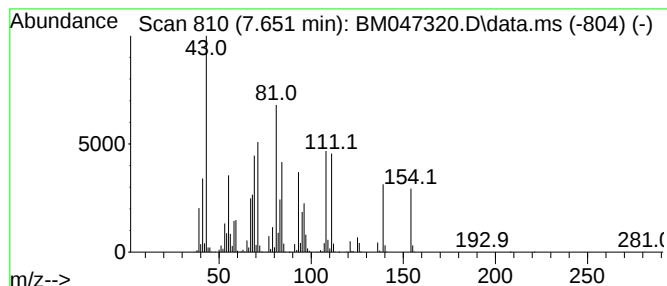
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.651	22.57 ng	1950690	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	59
3			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	35
4			3-Cyclohexen-1-ol, 4-methyl-1-(1...	154	C10H18O	020126-76-5	35
5			Terpinen-4-ol	154	C10H18O	000562-74-3	35



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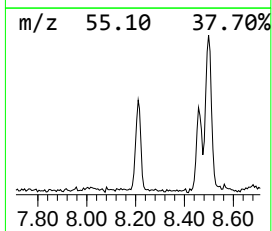
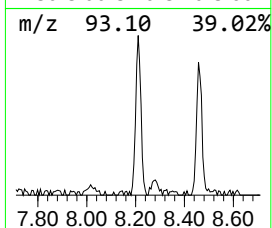
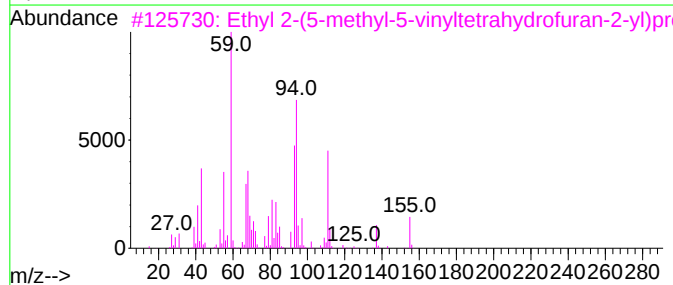
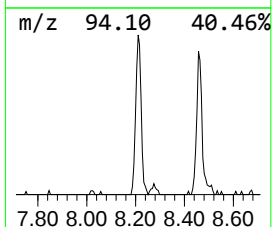
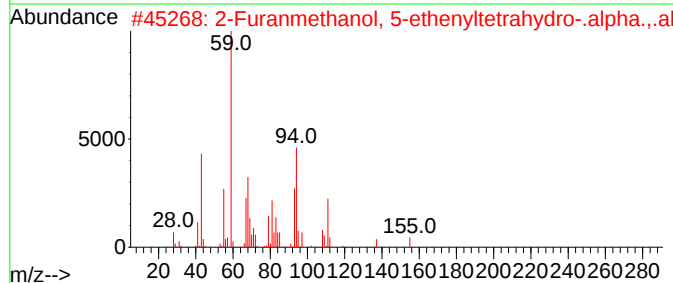
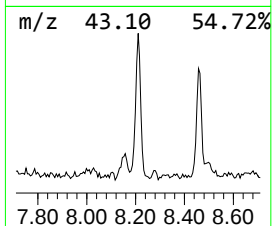
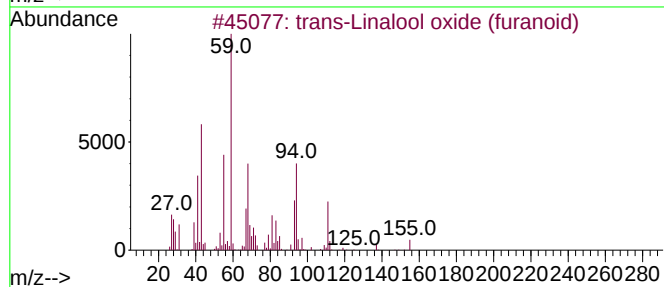
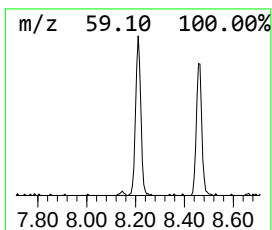
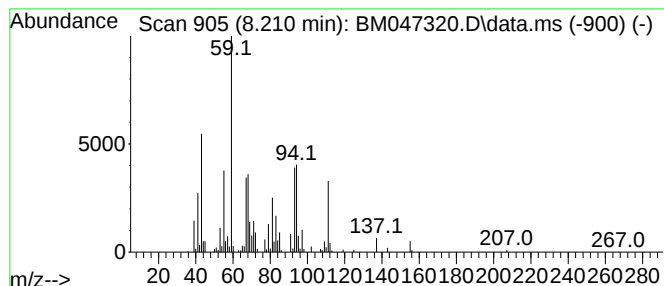
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 trans-Linalool oxide (furan... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.210	2.44 ng	210529	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Linalool oxide (furanoid)	170	C10H18O2	034995-77-2	80
2			2-Furanmethanol, 5-ethenyltetrahydro-	170	C10H18O2	005989-33-3	72
3			Ethyl 2-(5-methyl-5-vinyltetrahydro-	242	C13H22O4	1000373-80-3	68
4			cis-Linaloloxide	170	C10H18O2	1000121-97-4	49
5			.alpha.-Methyl-.alpha.-[4-methyl-	170	C10H18O2	1000132-13-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-911-KI-SO-0-0.5-081924

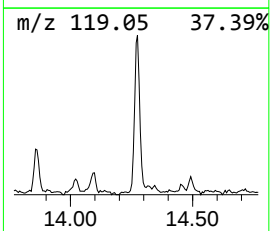
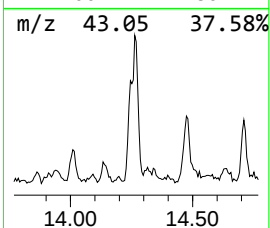
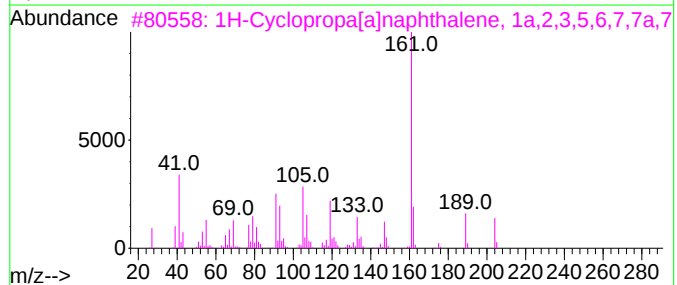
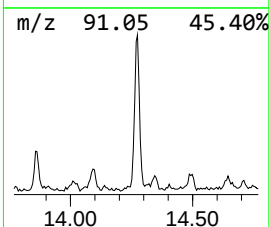
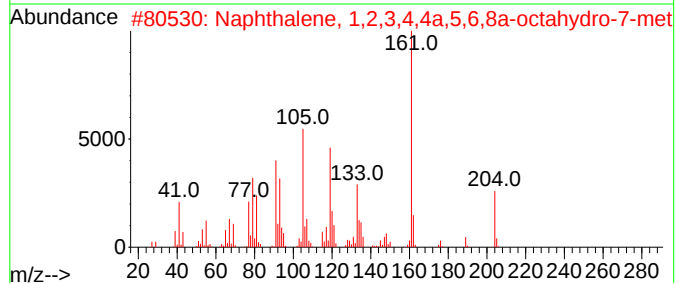
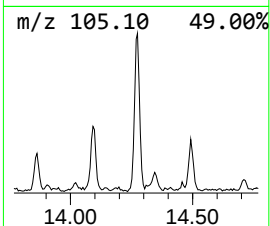
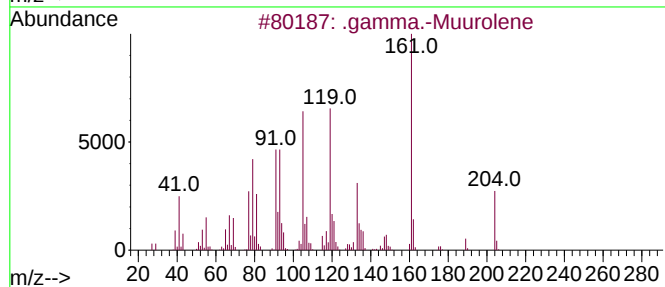
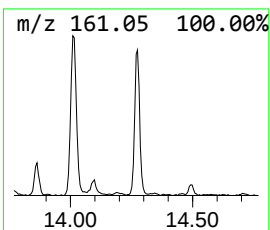
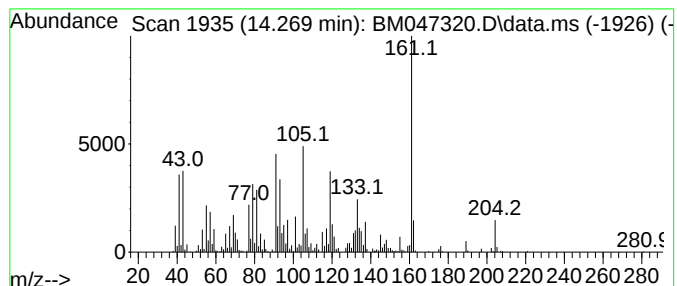
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 .gamma.-Muurolene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	4.06 ng	645796	Acenaphthene-d10	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Muurolene	204	C15H24	030021-74-0	98
2			Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	039029-41-9	96
3			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	91
4			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	86
5			(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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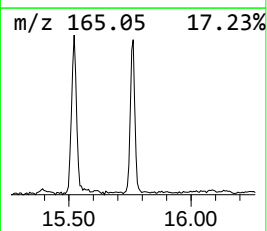
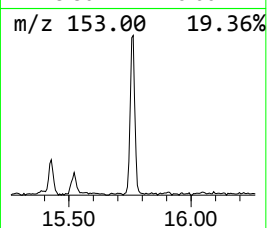
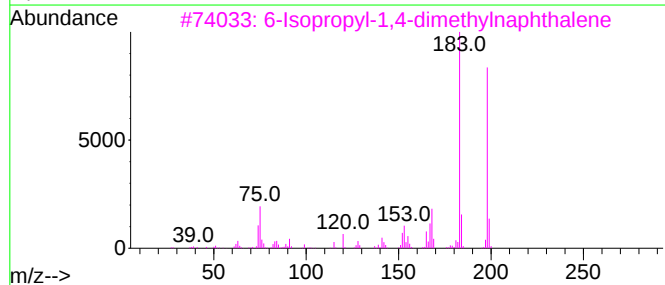
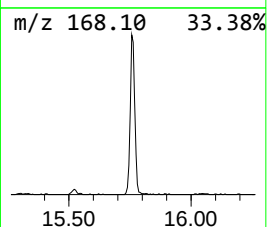
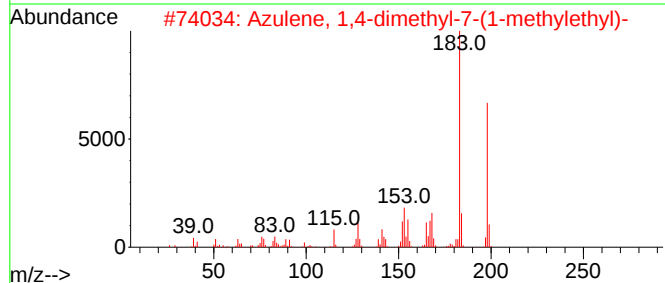
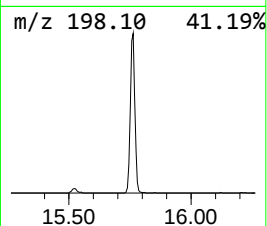
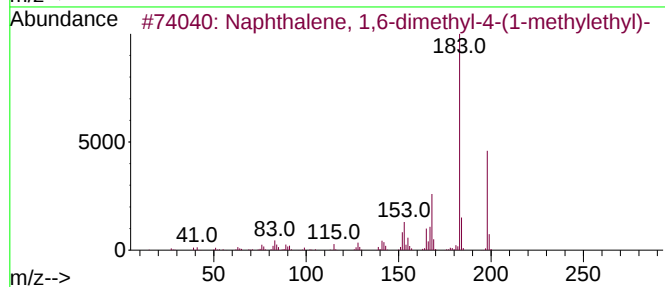
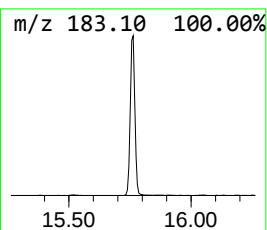
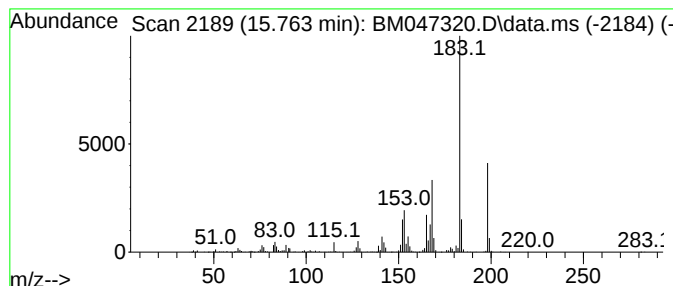
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, 1,6-dimethyl-4... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.763	2.82 ng	644628	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-4-(1-m...	198	C15H18	000483-78-3	98
2			Azulene, 1,4-dimethyl-7-(1-methy...	198	C15H18	000489-84-9	94
3			6-Isopropyl-1,4-dimethylnaphthalene	198	C15H18	000489-77-0	94
4			Cyclopropane, 1,1,2,2-tetramethy...	198	C15H18	1000264-08-5	72
5			Phenol, 2-(1-phenylethyl)-	198	C14H14O	004237-44-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
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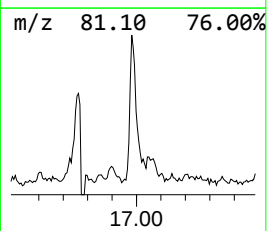
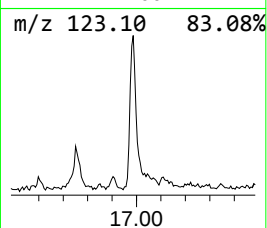
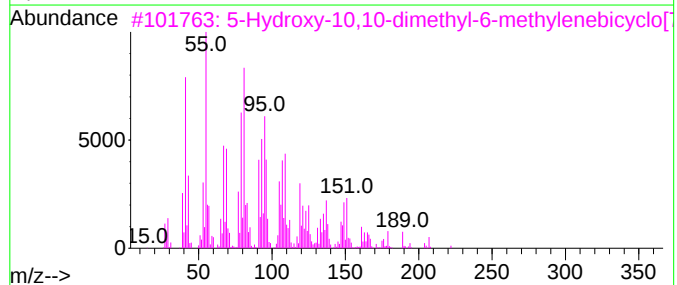
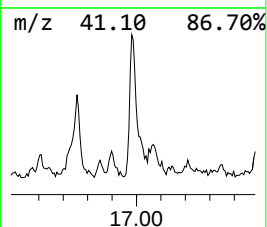
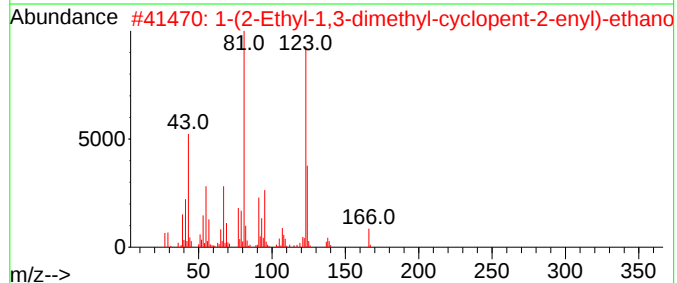
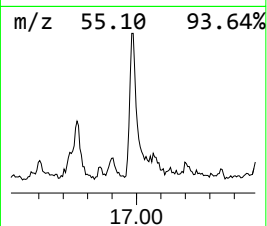
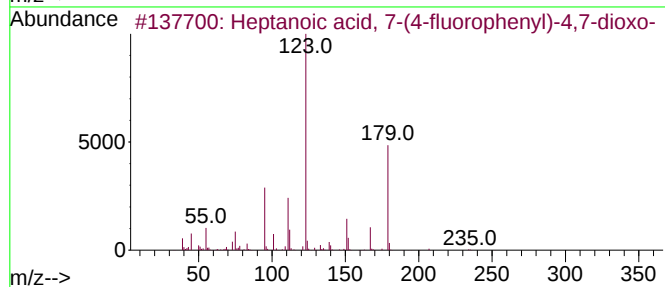
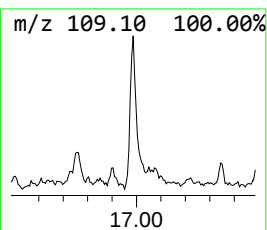
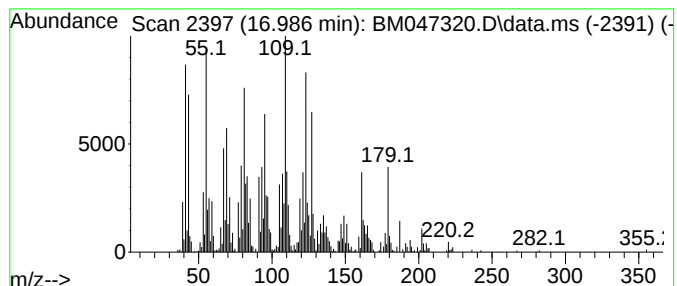
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown16.986 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.986	3.62 ng	826068	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanoic acid, 7-(4-fluoropheny...	252	C13H13F04	1010310-82-6	27
2			1-(2-Ethyl-1,3-dimethyl-cyclop...	166	C11H180	1010185-18-1	27
3			5-Hydroxy-10,10-dimethyl-6-methy...	222	C14H2202	096480-63-6	22
4			Cyclohexanol, 3-ethenyl-3-methyl...	222	C15H260	035727-45-8	22
5			(4E,8E,13E)-1-(2-Hydroxyethyl)-1...	276	C19H320	1000426-96-0	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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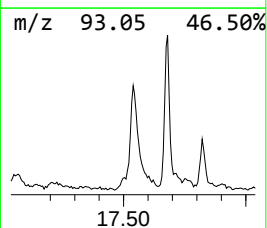
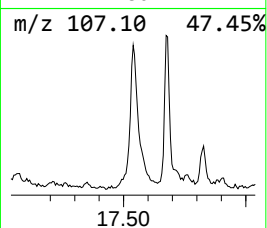
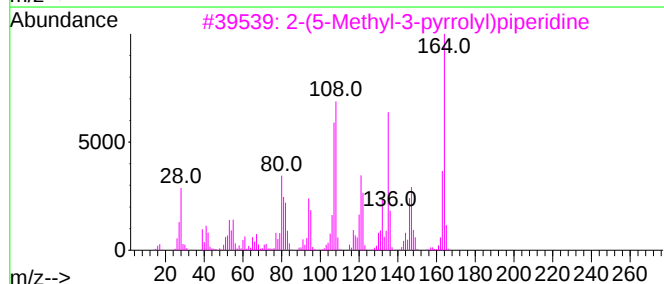
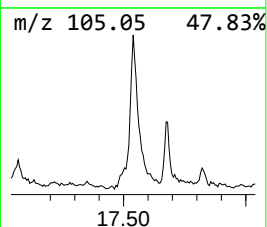
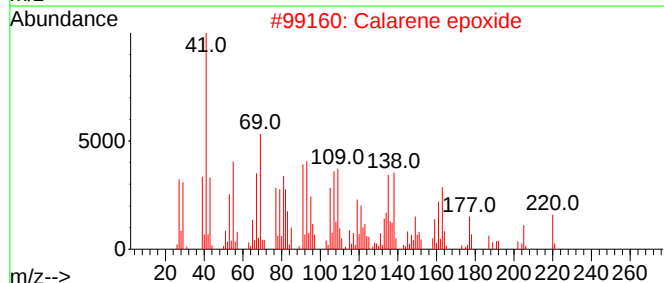
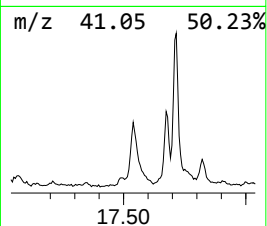
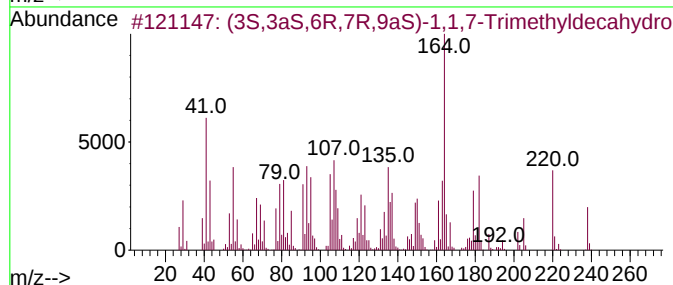
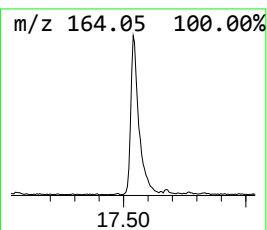
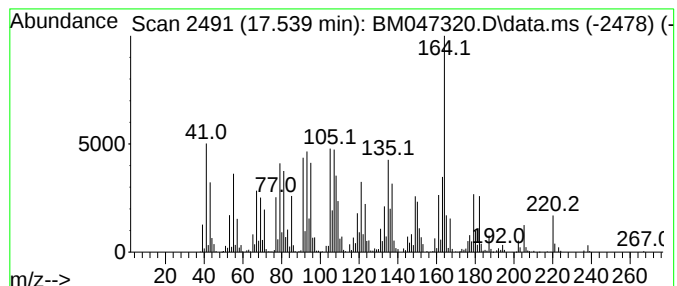
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 (3S,3aS,6R,7R,9aS)-1,1,7-Tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.539	8.89 ng	2030630	Phenanthrene-d10	16.774

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(3S,3aS,6R,7R,9aS)-1,1,7-Trimeth...	238	C15H26O2	002649-64-1	99
2		Calarene epoxide	220	C15H24O	1000151-46-0	46
3		2-(5-Methyl-3-pyrrolyl)piperidine	164	C10H16N2	1000245-18-2	38
4		5-Pyrrolidin-2-ylidenemethyl-3,4...	164	C9H12N2O	1010192-09-5	35
5		5-Methoxy-2-allylphenol	164	C10H12O2	1000306-52-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
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Instrument :
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ClientSampleId :
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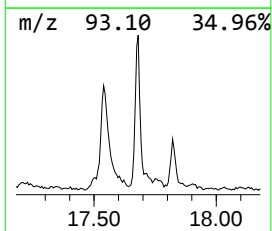
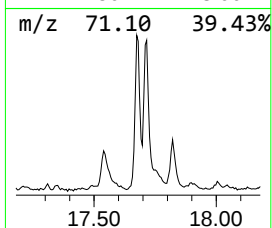
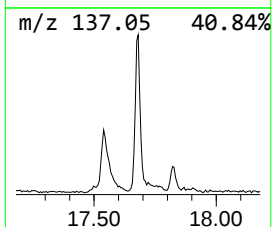
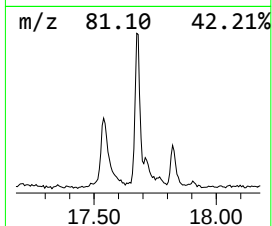
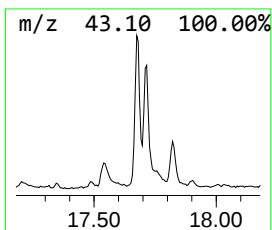
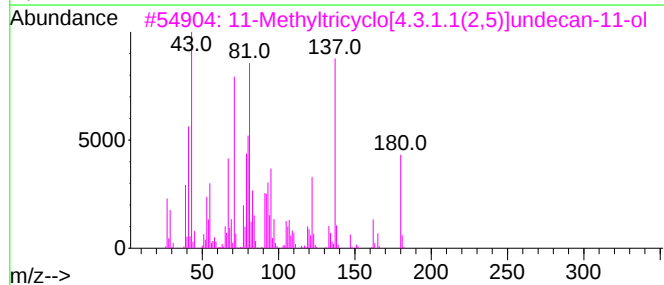
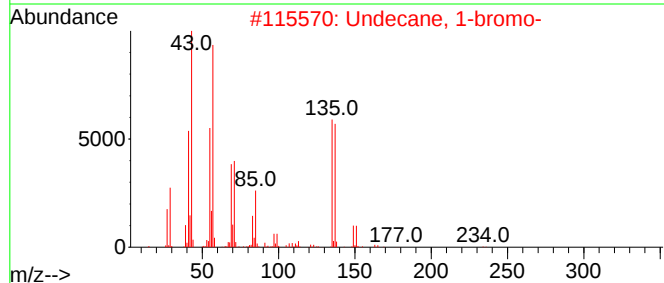
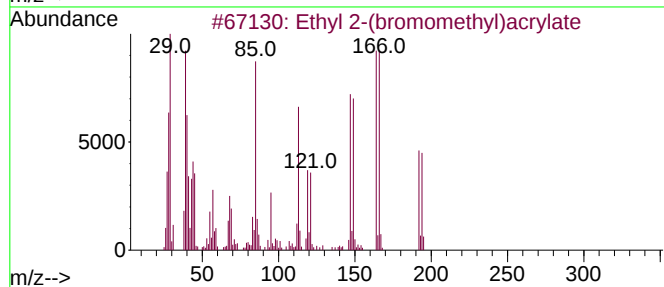
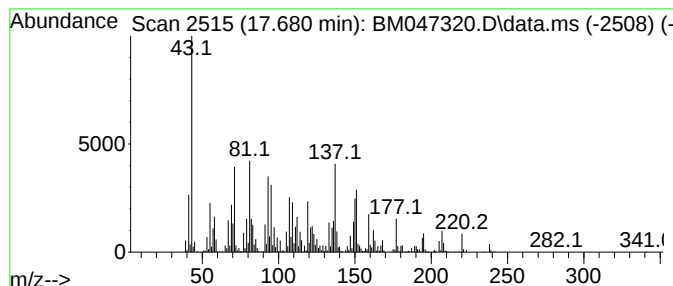
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Ethyl 2-(bromomethyl)acrylate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.680	6.58 ng	1501840	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl 2-(bromomethyl)acrylate	192	C6H9BrO2	017435-72-2	90
2			Undecane, 1-bromo-	234	C11H23Br	000693-67-4	38
3			11-Methyltricyclo[4.3.1.1(2,5)]u...	180	C12H20O	174226-52-9	25
4			Pentane, 1,1'-sulfonylbis-	206	C10H22O2S	004253-99-0	16
5			(1-Cyclopropylimidazol-2-yl)meth...	137	C7H11N3	1000444-19-0	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
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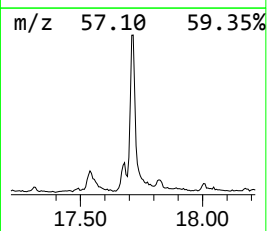
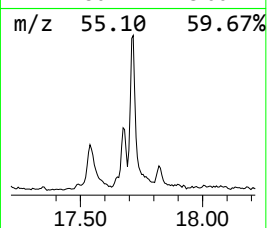
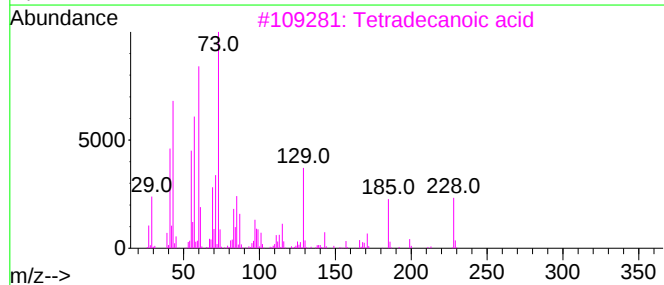
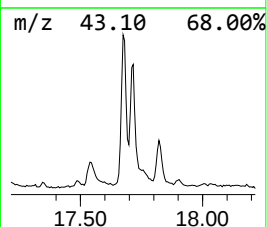
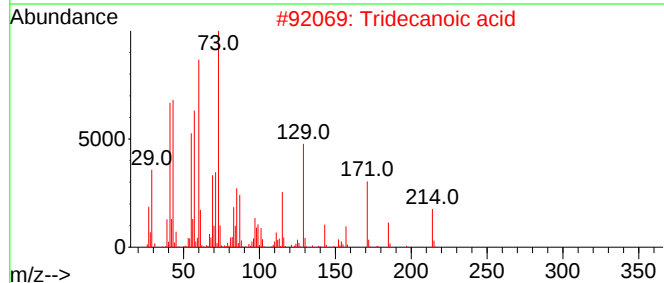
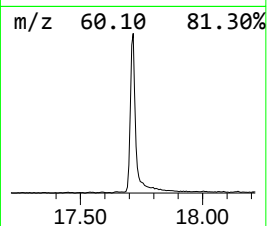
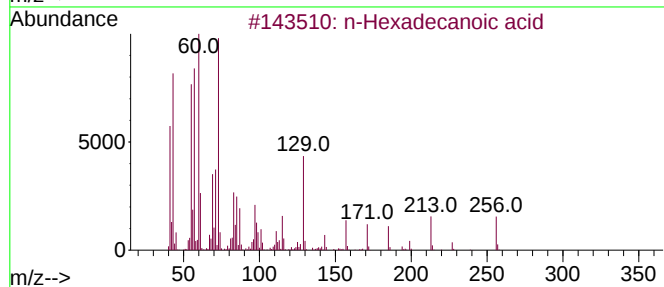
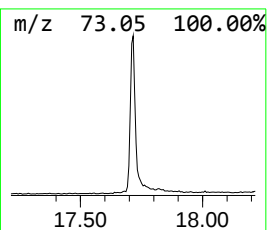
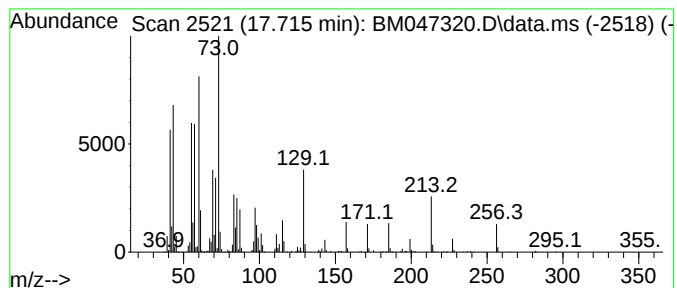
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	4.92 ng	1122560	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Octadecanoic acid	284	C18H36O2	000057-11-4	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
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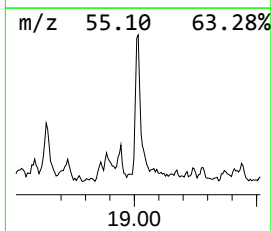
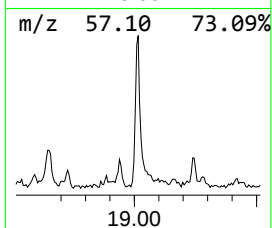
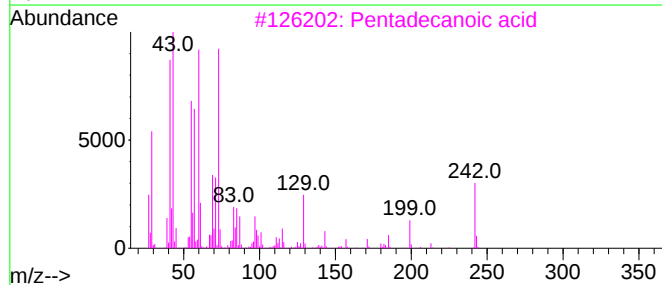
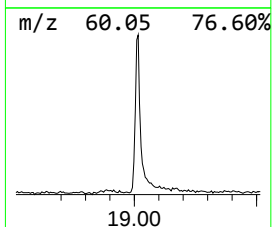
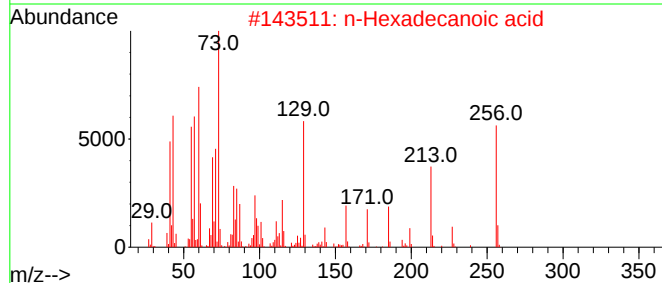
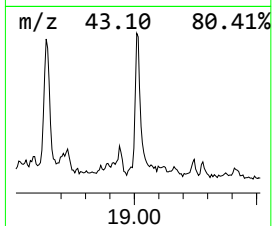
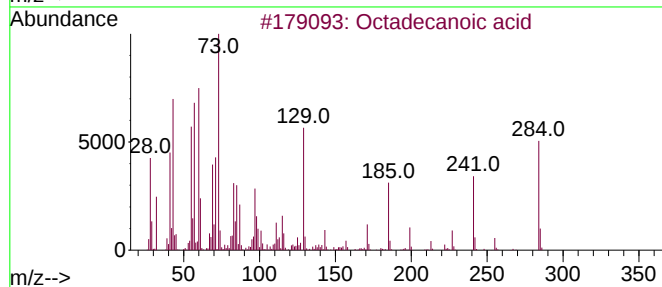
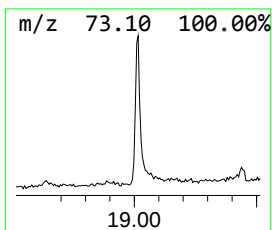
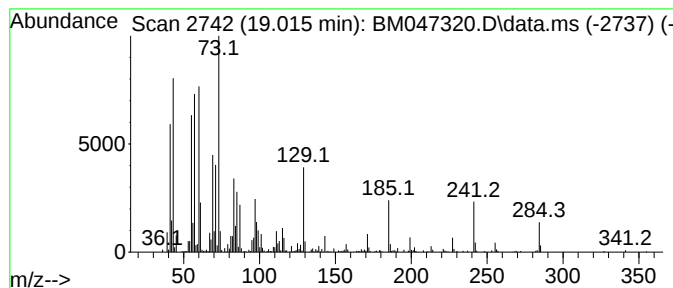
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octadecanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	3.09 ng	533544	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-911-KI-SO-0-0.5-081924

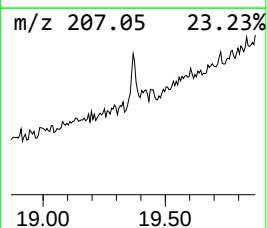
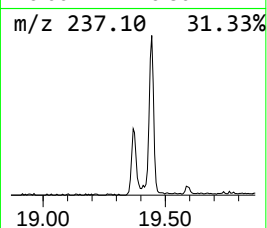
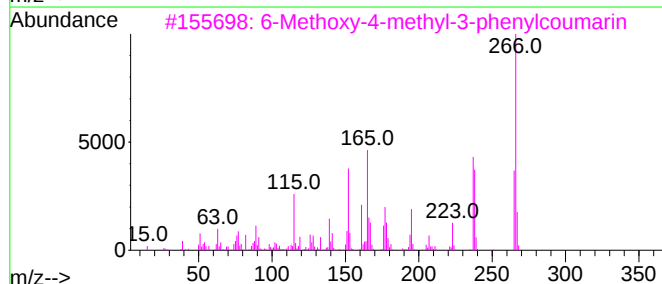
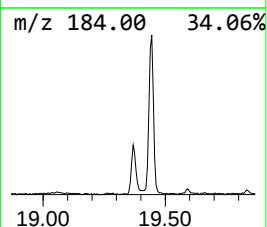
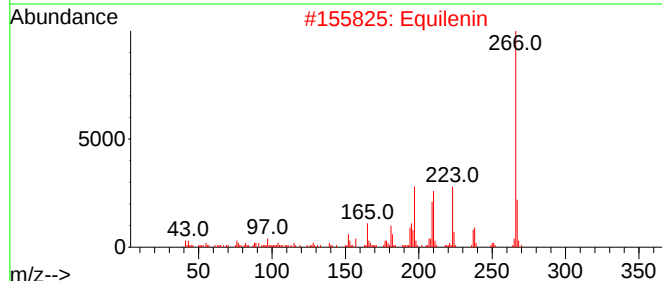
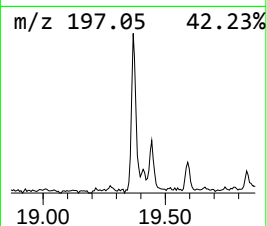
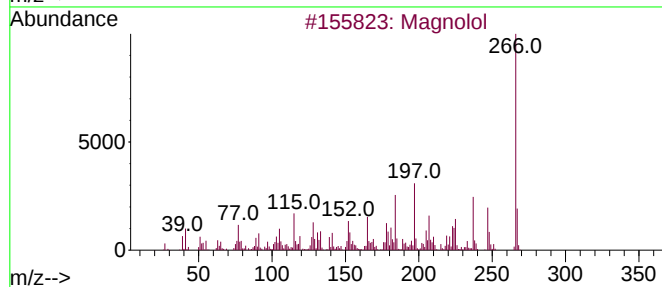
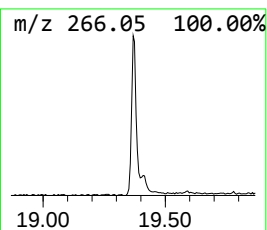
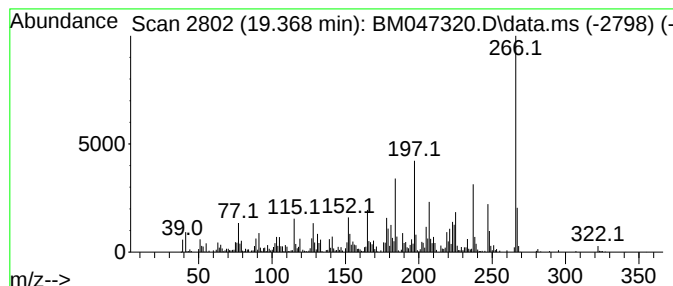
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Magnolol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.368	2.86 ng	495158	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Magnolol	266	C18H18O2	000528-43-8	99
2			Equilenin	266	C18H18O2	000517-09-9	46
3			6-Methoxy-4-methyl-3-phenylcoumarin	266	C17H14O3	115059-27-3	43
4			5,5'-Diallyl-2,2'-biphenyldiol d...	350	C22H22O4	1000384-18-2	43
5			Benzo[1mn][3,8]phenanthroline-1,...	266	C14H6N2O4	005690-24-4	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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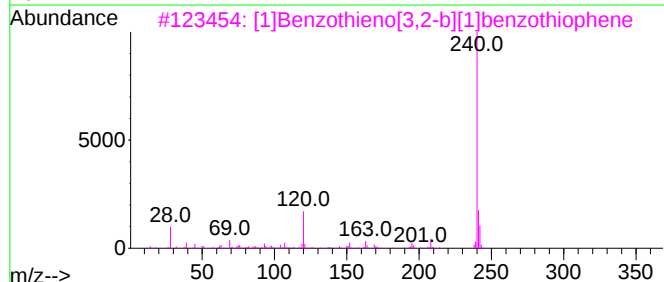
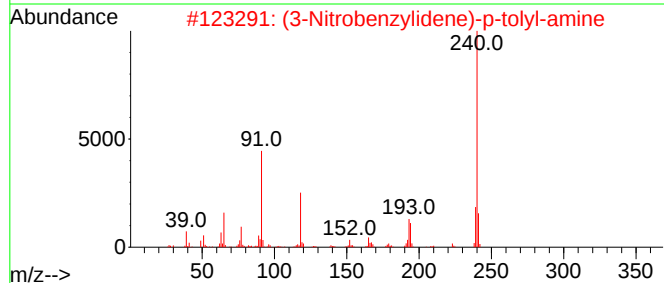
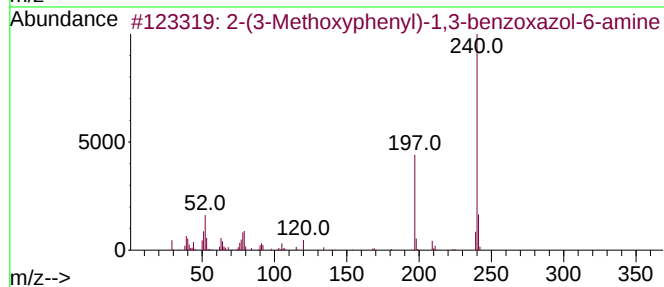
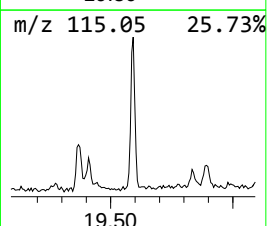
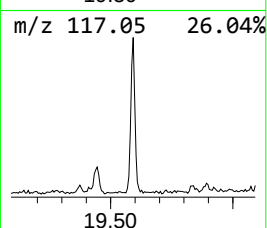
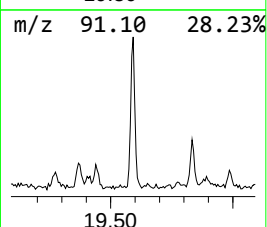
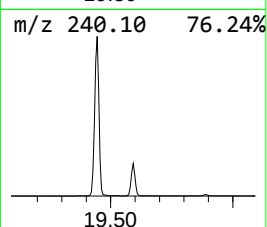
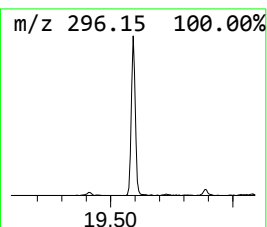
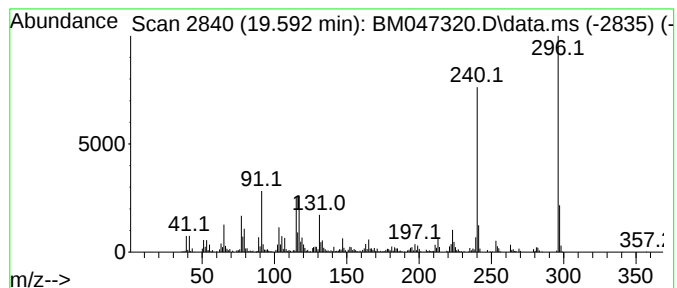
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown19.592 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.592	3.51 ng	606155	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(3-Methoxyphenyl)-1,3-benzoxaz...	240	C14H12N2O2	1000444-16-7	38		
2	(3-Nitrobenzylidene)-p-tolyl-amine	240	C14H12N2O2	000730-39-2	38		
3	[1]Benzothieno[3,2-b][1]benzothi...	240	C14H8S2	000248-70-4	38		
4	Dibenzo[a,c]phenazin-10-ol	296	C20H12N2O	1000300-08-6	38		
5	1,4-Dithiin, 2,5-bis(4-methylphe...	296	C18H16S2	037989-48-3	30		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
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Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
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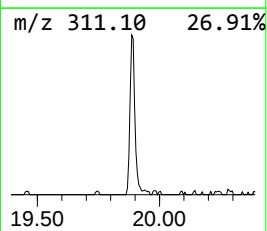
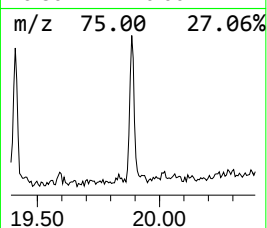
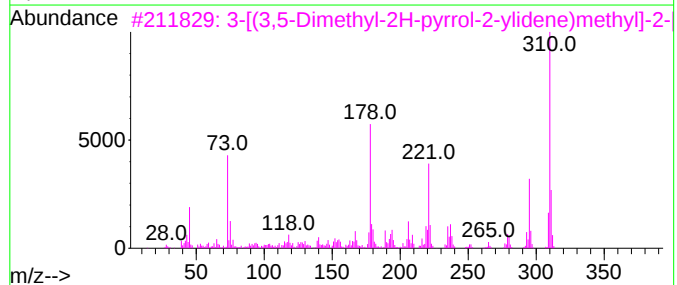
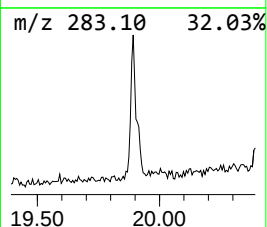
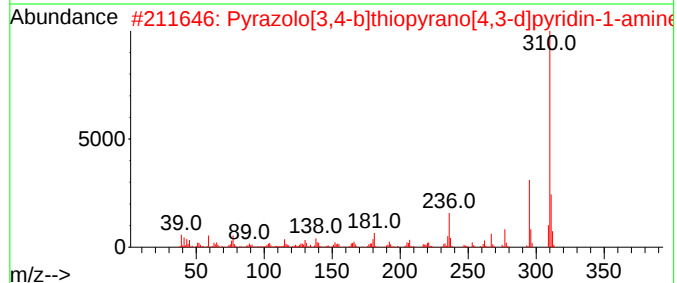
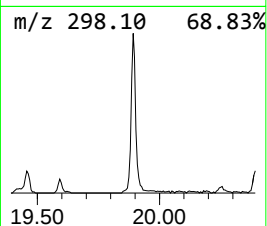
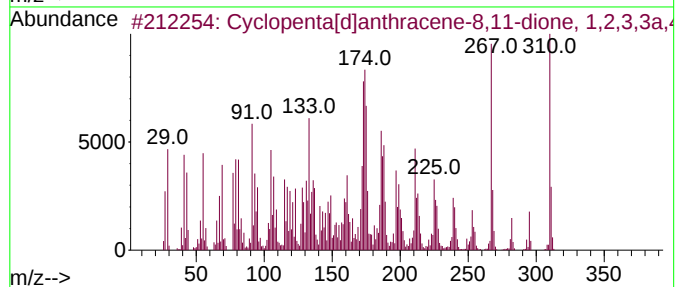
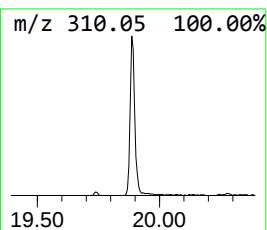
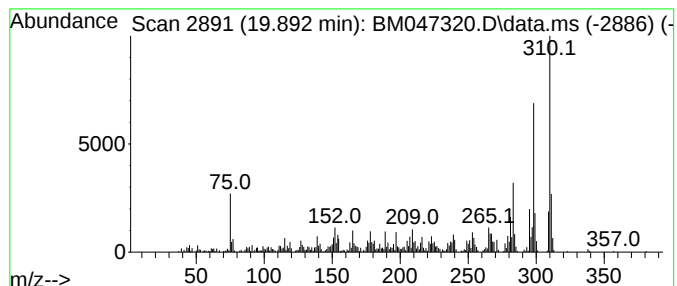
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Cyclopenta[d]anthracene-8,11-dione Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.892	3.16 ng	545709	Chrysene-d12	21.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta[d]anthracene-8,11-dio...	310	C21H26O2	1010188-44-2	95
2	Pyrazolo[3,4-b]thiopyrano[4,3-d]...	310	C17H18N4S	303051-16-3	70
3	3-[(3,5-Dimethyl-2H-pyrrol-2-yl)...	310	C18H22N2OSi	1000408-37-5	64
4	3-(3',4'-Dimethoxyphenyl)-4,6-di...	310	C19H18O4	720674-12-4	55
5	(3aR,10aS)-7-(4-Methoxyphenyl)-3...	310	C20H22O3	1000482-62-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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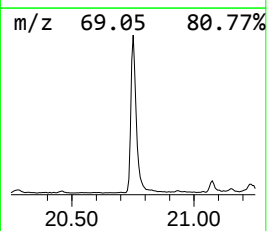
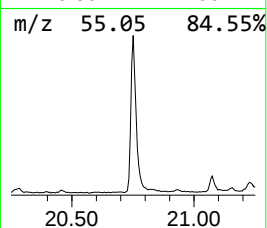
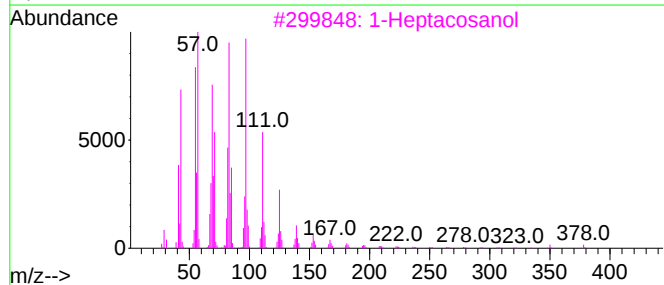
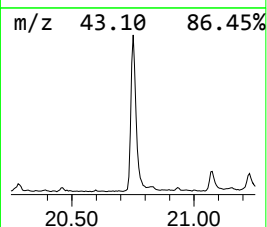
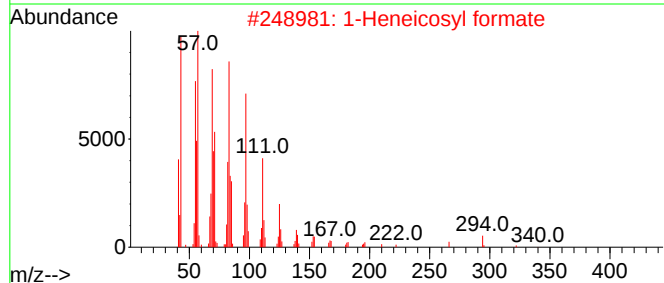
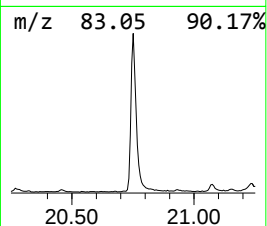
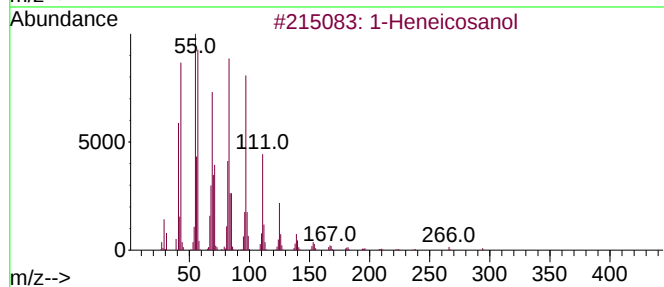
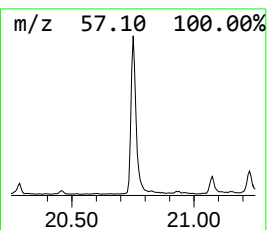
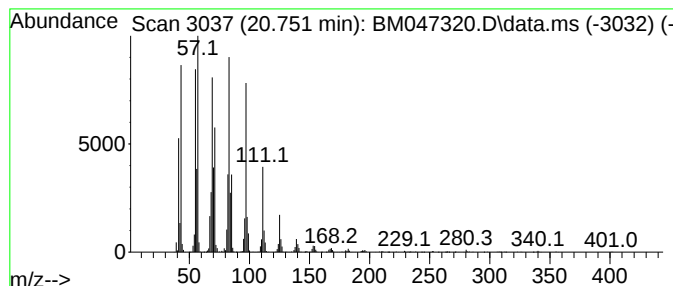
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.751	16.85 ng	2913150	Chrysene-d12	21.015

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	93
4		1-Tetracosene	336	C24H48	010192-32-2	91
5		1-Hexacosanol	382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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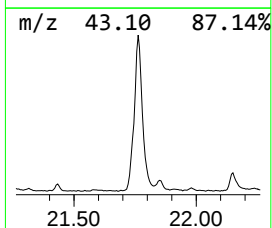
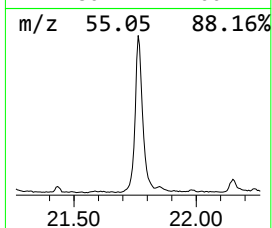
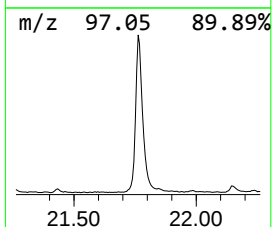
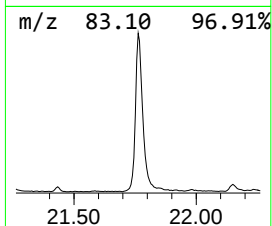
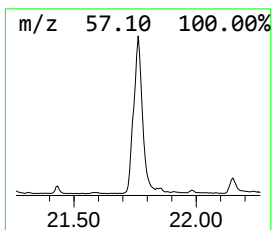
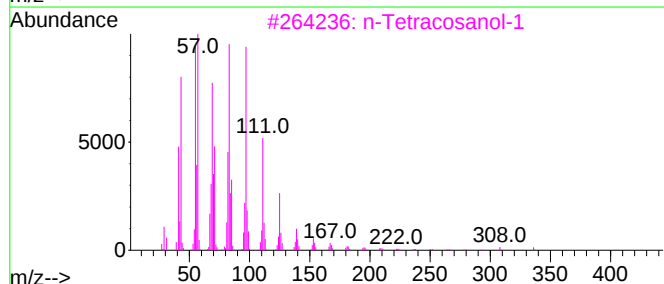
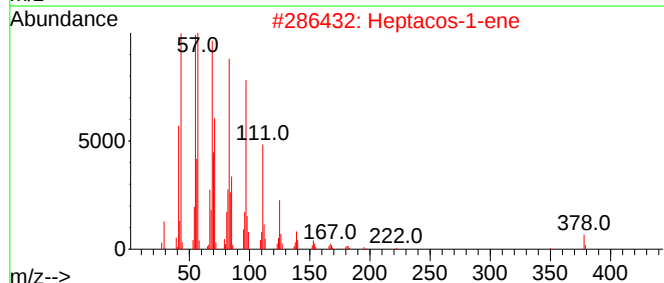
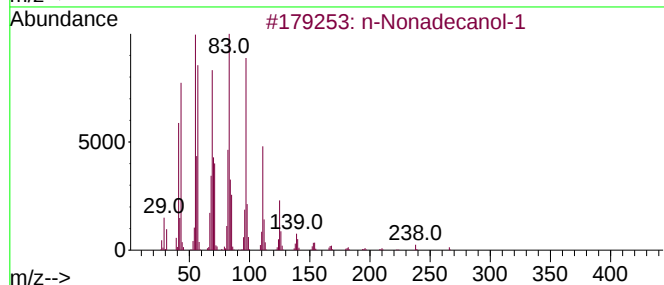
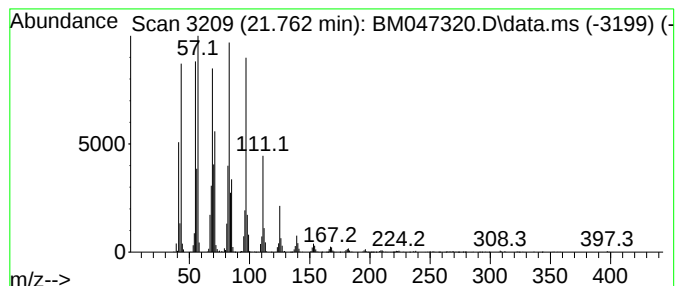
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 n-Nonadecanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.
21.762	29.24 ng	5056030	Chrysene-d12		21.015

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94	
2	Heptacos-1-ene	378	C27H54	015306-27-1	94	
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94	
4	Pentacos-1-ene	350	C25H50	016980-85-1	94	
5	1-Heneicosanol	312	C21H44O	015594-90-8	94	



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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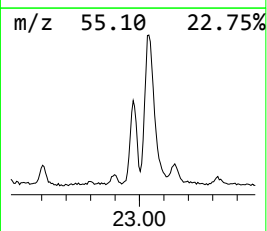
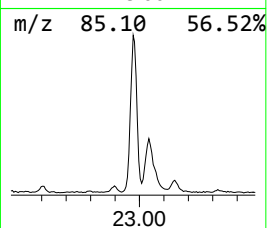
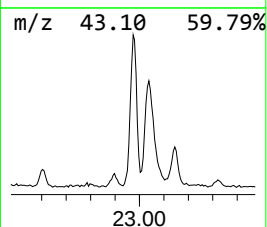
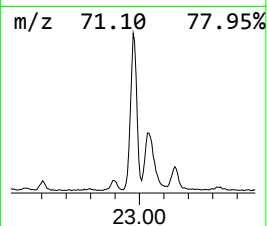
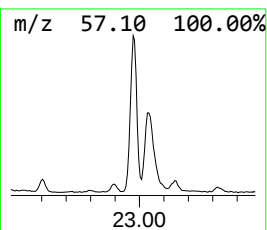
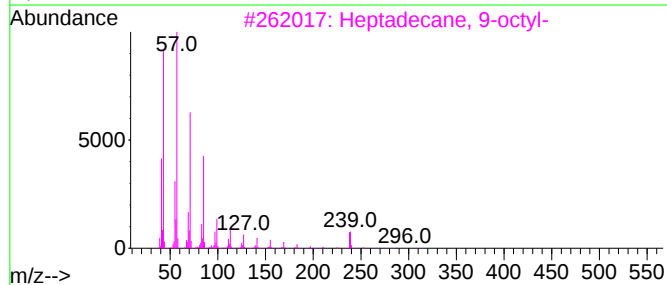
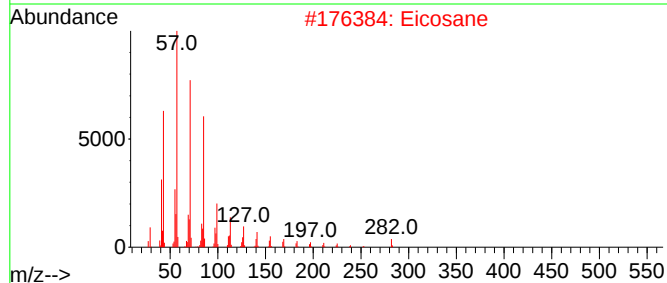
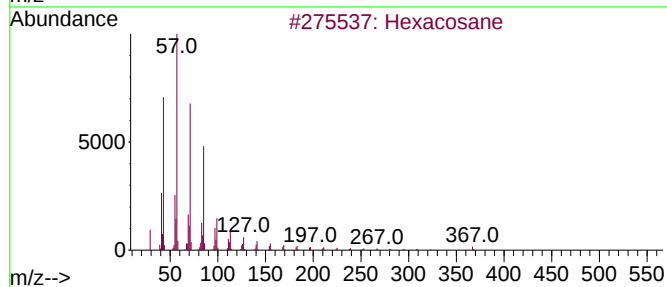
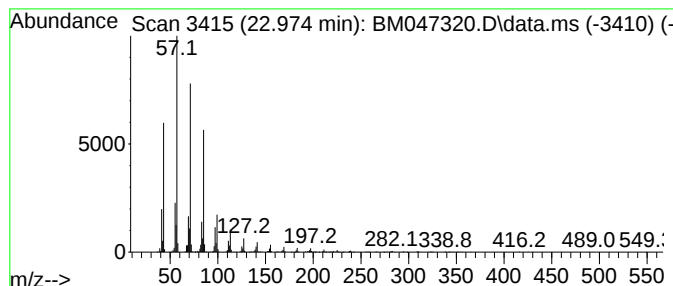
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.974	6.83 ng	1115230	Perylene-d12	23.709

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	94
2		Eicosane	282	C20H42	000112-95-8	94
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
4		Octacosane	394	C28H58	000630-02-4	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-911-KI-SO-0-0.5-081924

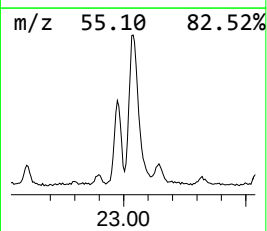
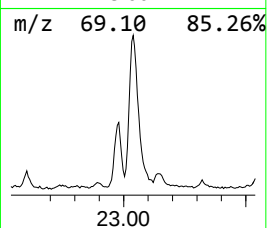
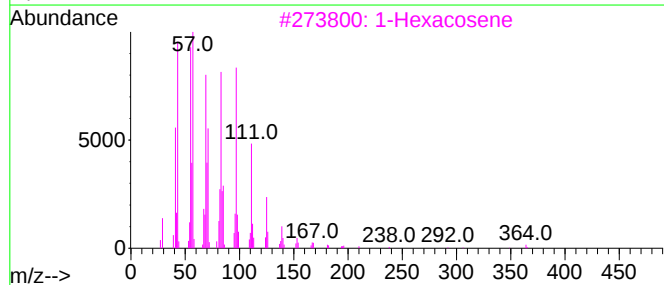
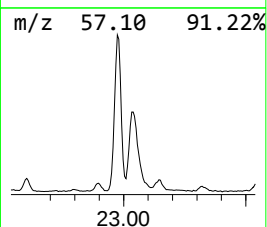
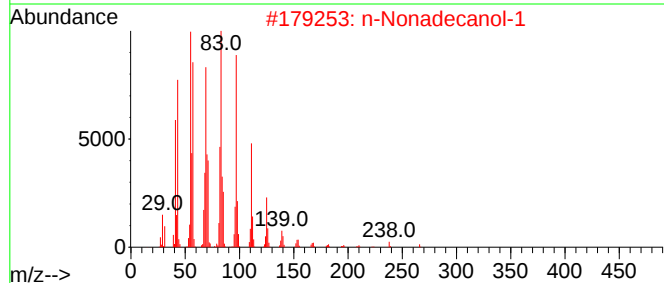
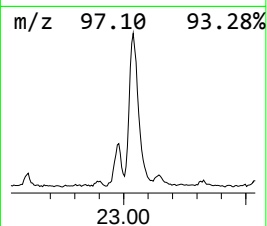
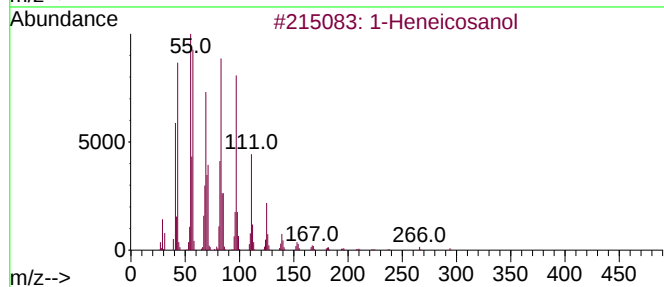
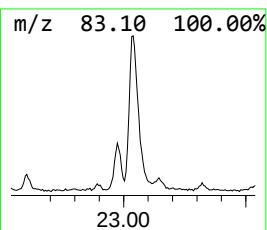
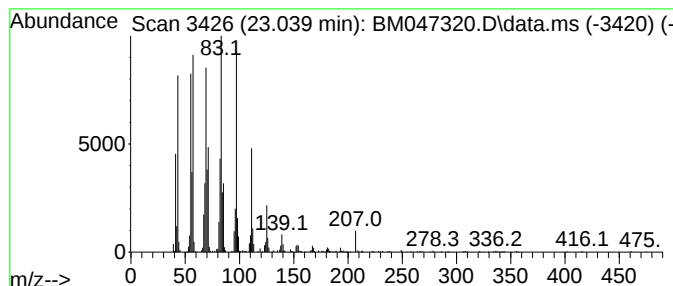
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 1-Hexacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.039	10.37 ng	1693470	Perylene-d12	23.709

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3		1-Hexacosene	364	C26H52	018835-33-1	91
4		Octacosanol	410	C28H58O	000557-61-9	91
5		1-Tetracosene	336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-911-KI-SO-0-0.5-081924

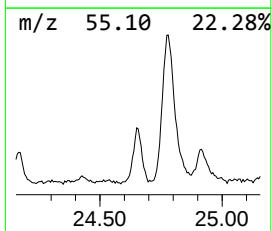
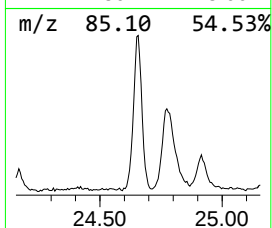
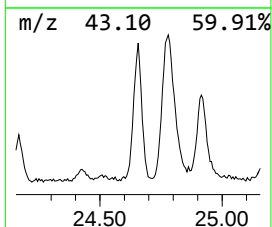
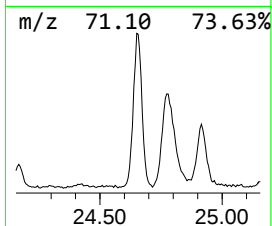
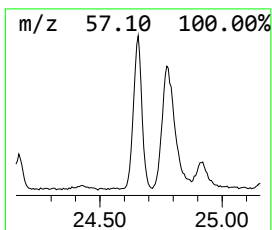
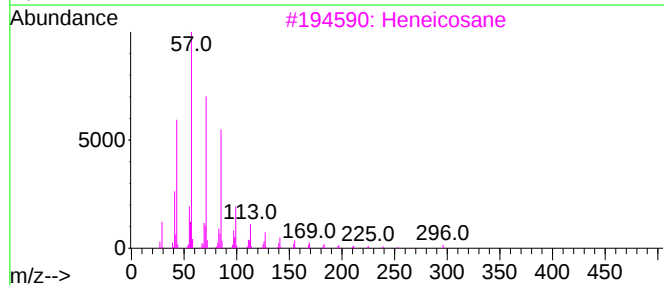
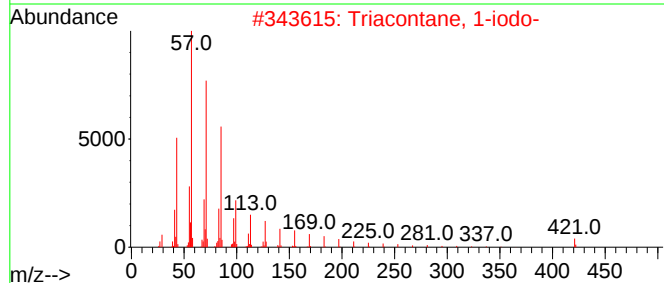
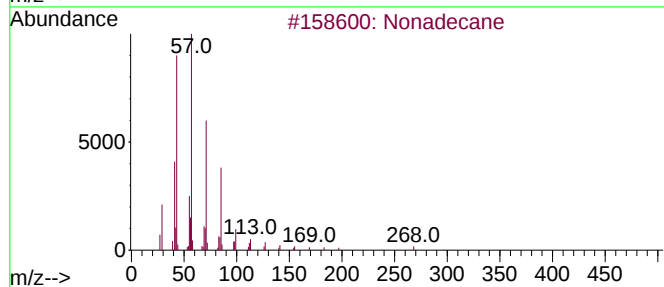
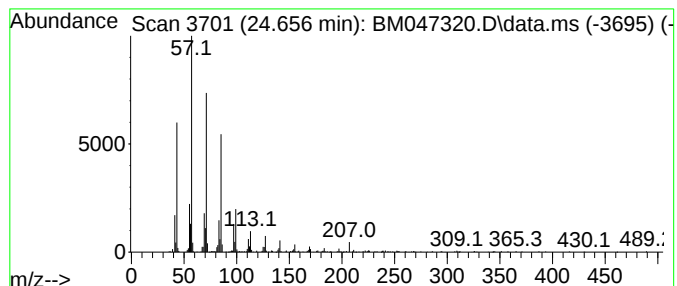
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.656	5.05 ng	824710	Perylene-d12	23.709

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	95
2		Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5		Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-911-KI-SO-0-0.5-081924

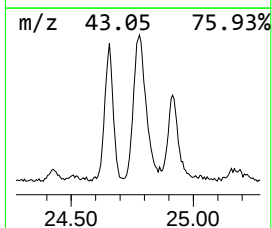
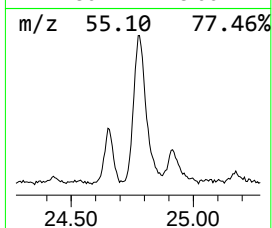
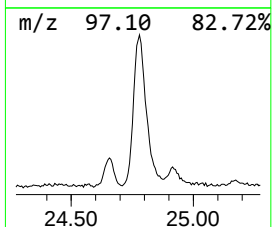
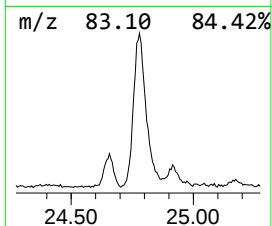
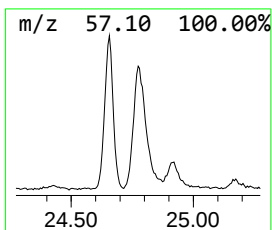
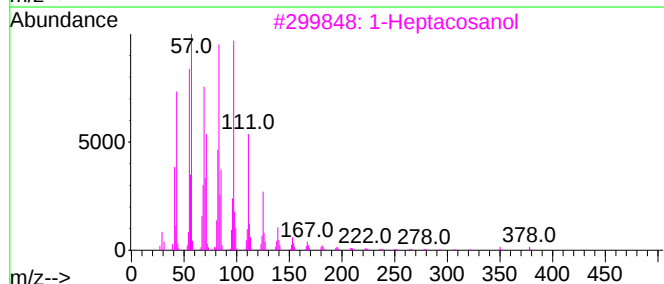
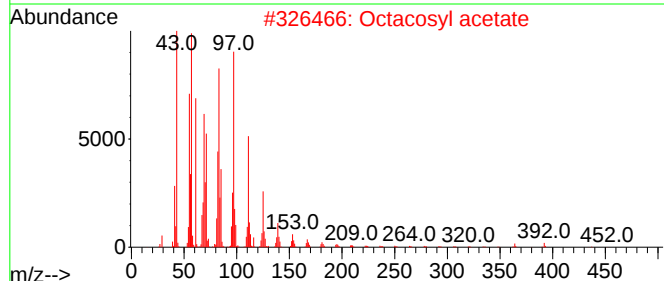
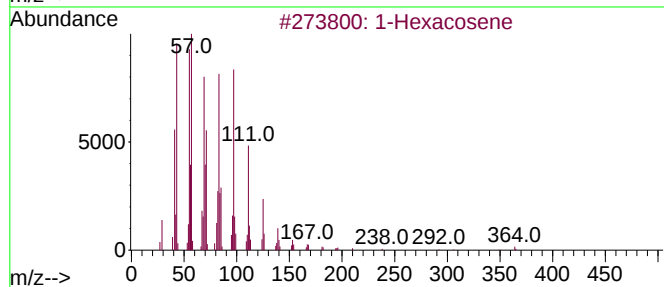
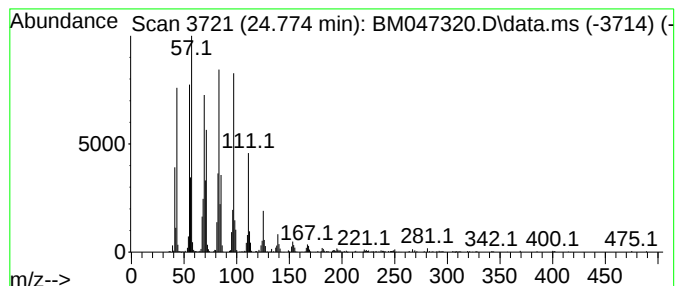
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Octacosyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.774	11.53 ng	1881960	Perylene-d12	23.709

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	95
2	Octacosyl acetate			452	C30H60O2	018206-97-8	95
3	1-Heptacosanol			396	C27H56O	002004-39-9	95
4	1-Heneicosanol			312	C21H44O	015594-90-8	93
5	Octacosanol			410	C28H58O	000557-61-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082224\
Data File : BM047320.D
Acq On : 22 Aug 2024 17:10
Operator : RC/JU
Sample : P3671-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-911-KI-SO-0-0.5-081924

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	4.563	3.5	ng	298712	1	7.351	1728750	20.0
Eucalyptol	7.651	22.6	ng	1950690	1	7.351	1728750	20.0
trans-Linalool ...	8.210	2.4	ng	210529	1	7.351	1728750	20.0
.gamma.-Muurolene	14.269	4.1	ng	645796	3	14.010	3181900	20.0
Naphthalene, 1,...	15.763	2.8	ng	644628	4	16.774	4566080	20.0
unknown16.986	16.986	3.6	ng	826068	4	16.774	4566080	20.0
(3S,3aS,6R,7R,9...	17.539	8.9	ng	2030630	4	16.774	4566080	20.0
Ethyl 2-(bromom...	17.680	6.6	ng	1501840	4	16.774	4566080	20.0
n-Hexadecanoic ...	17.715	4.9	ng	1122560	4	16.774	4566080	20.0
Octadecanoic acid	19.015	3.1	ng	533544	5	21.015	3458660	20.0
Magnolol	19.368	2.9	ng	495158	5	21.015	3458660	20.0
unknown19.592	19.592	3.5	ng	606155	5	21.015	3458660	20.0
Cyclopenta[d]an...	19.892	3.2	ng	545709	5	21.015	3458660	20.0
1-Heneicosanol	20.751	16.9	ng	2913150	5	21.015	3458660	20.0
n-Nonadecanol-1	21.762	29.2	ng	5056030	5	21.015	3458660	20.0
Hexacosane	22.974	6.8	ng	1115230	6	23.709	3265220	20.0
1-Hexacosene	23.039	10.4	ng	1693470	6	23.709	3265220	20.0
Nonadecane	24.656	5.0	ng	824710	6	23.709	3265220	20.0
Octacosyl acetate	24.774	11.5	ng	1881960	6	23.709	3265220	20.0