

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
 Data File : BM046349.D
 Acq On : 28 Jun 2024 12:46
 Operator : MA/JU
 Sample : P3076-10
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 7-S-1

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-BM062724.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046349.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.293	66	69	85	rBV	54141	116209	2.55%	0.363%
2	4.593	285	290	301	rBV	117402	196878	4.31%	0.616%
3	5.046	361	367	389	rBV	1849947	2924954	64.10%	9.146%
4	6.628	629	636	659	rBV	1675808	3113396	68.23%	9.735%
5	7.369	756	762	778	rBV	512694	856279	18.77%	2.678%
6	8.540	953	961	982	rBV	883821	1943228	42.59%	6.076%
7	9.222	1069	1077	1086	rBV4	14457	45672	1.00%	0.143%
8	10.139	1225	1233	1255	rBV	508776	1114400	24.42%	3.485%
9	10.945	1363	1370	1384	rBV2	46239	136756	3.00%	0.428%
10	12.639	1651	1658	1677	rBV	1905112	3273386	71.74%	10.236%
11	14.022	1886	1893	1911	rBV	834566	1369936	30.02%	4.284%
12	14.304	1938	1941	1949	rVB	39421	61699	1.35%	0.193%
13	15.527	2142	2149	2165	rBV	2042158	3262879	71.51%	10.203%
14	16.774	2355	2361	2367	rBV	945952	1513074	33.16%	4.731%
15	16.921	2382	2386	2394	rVB3	32222	66174	1.45%	0.207%
16	17.145	2411	2424	2434	rBV6	37260	168077	3.68%	0.526%
17	17.710	2514	2520	2540	rBV	546693	1214513	26.62%	3.798%
18	18.698	2682	2688	2700	rVB4	52533	143807	3.15%	0.450%
19	18.845	2709	2713	2728	rBV	171173	307828	6.75%	0.963%
20	18.998	2734	2739	2752	rBV	228297	511525	11.21%	1.599%
21	19.209	2768	2775	2779	rBV	139688	204315	4.48%	0.639%
22	19.421	2806	2811	2824	rBV	3795184	4562858	100.00%	14.268%
23	19.745	2858	2866	2875	rVB2	119845	227429	4.98%	0.711%
24	20.245	2947	2951	2955	rBV4	47782	61044	1.34%	0.191%
25	20.551	2999	3003	3011	rVB	122086	163171	3.58%	0.510%
26	20.709	3026	3030	3039	rBV2	192471	368902	8.08%	1.154%
27	20.992	3072	3078	3083	rBV	1003014	1510881	33.11%	4.724%
28	21.168	3106	3108	3114	rVB2	63017	75450	1.65%	0.236%
29	21.292	3125	3129	3135	rVB	85102	144132	3.16%	0.451%
30	21.674	3191	3194	3198	rBV2	65298	88431	1.94%	0.277%
31	21.962	3236	3243	3257	rVB3	171465	537945	11.79%	1.682%
32	22.239	3287	3290	3296	rVB	71244	99695	2.18%	0.312%
33	22.403	3314	3318	3324	rVB	137968	212551	4.66%	0.665%
34	23.662	3526	3532	3549	rVB	591903	1383043	30.31%	4.325%

Sum of corrected areas: 31980517

Instrument :

BNA_M

ClientSampleId :

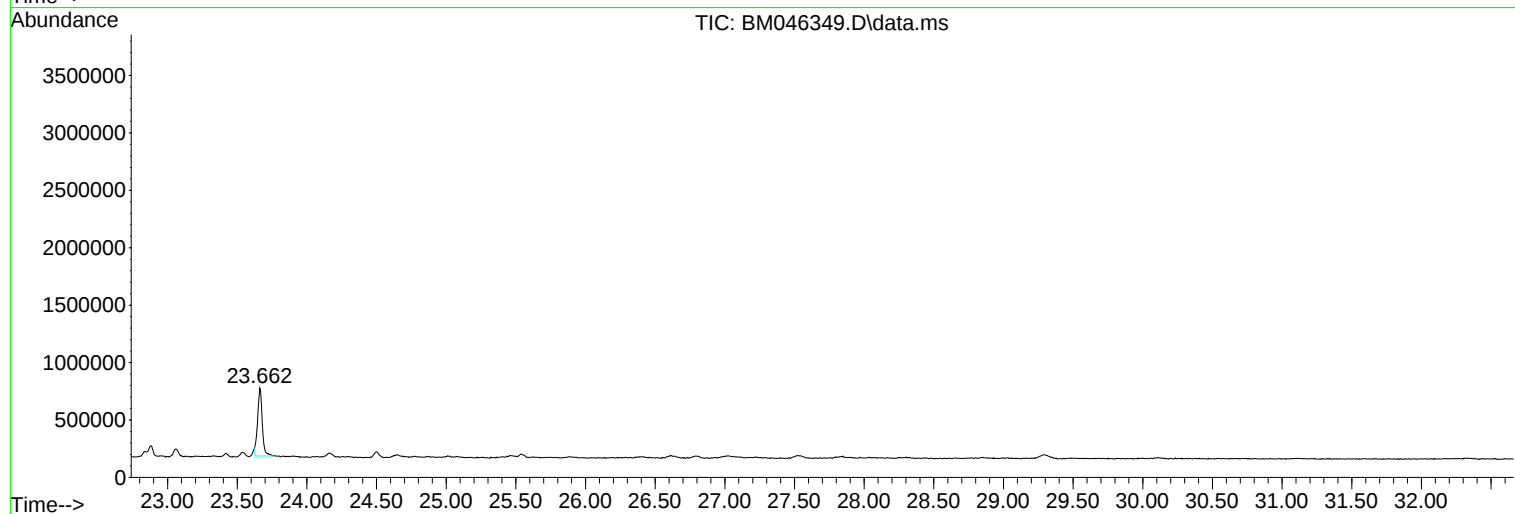
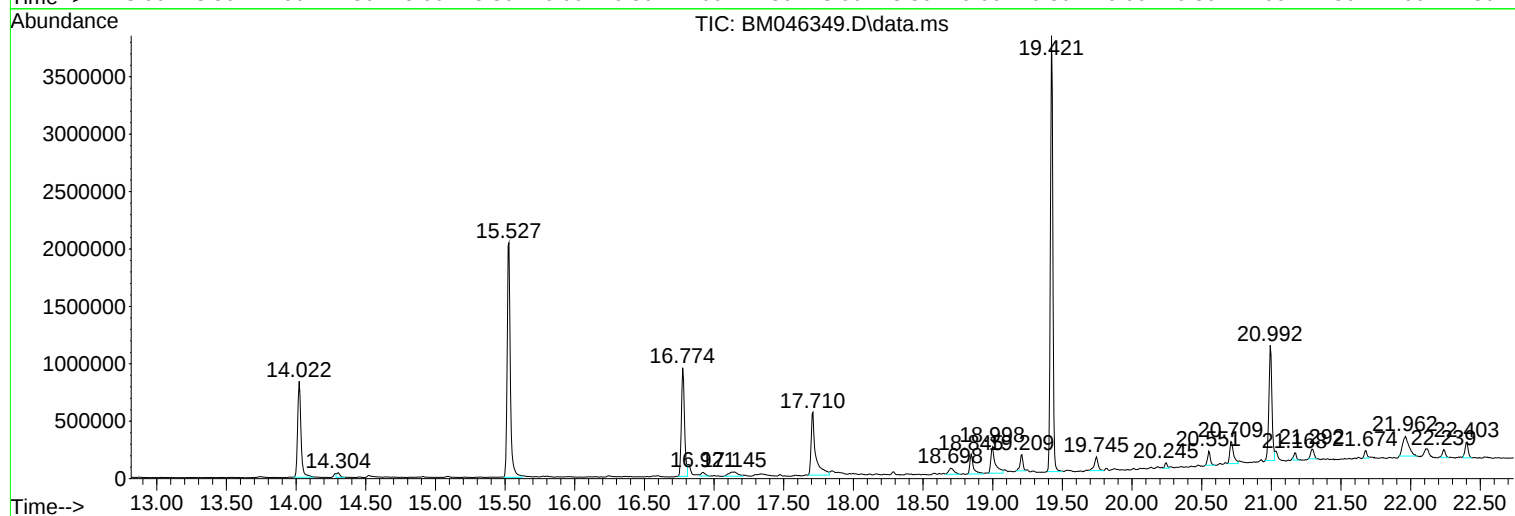
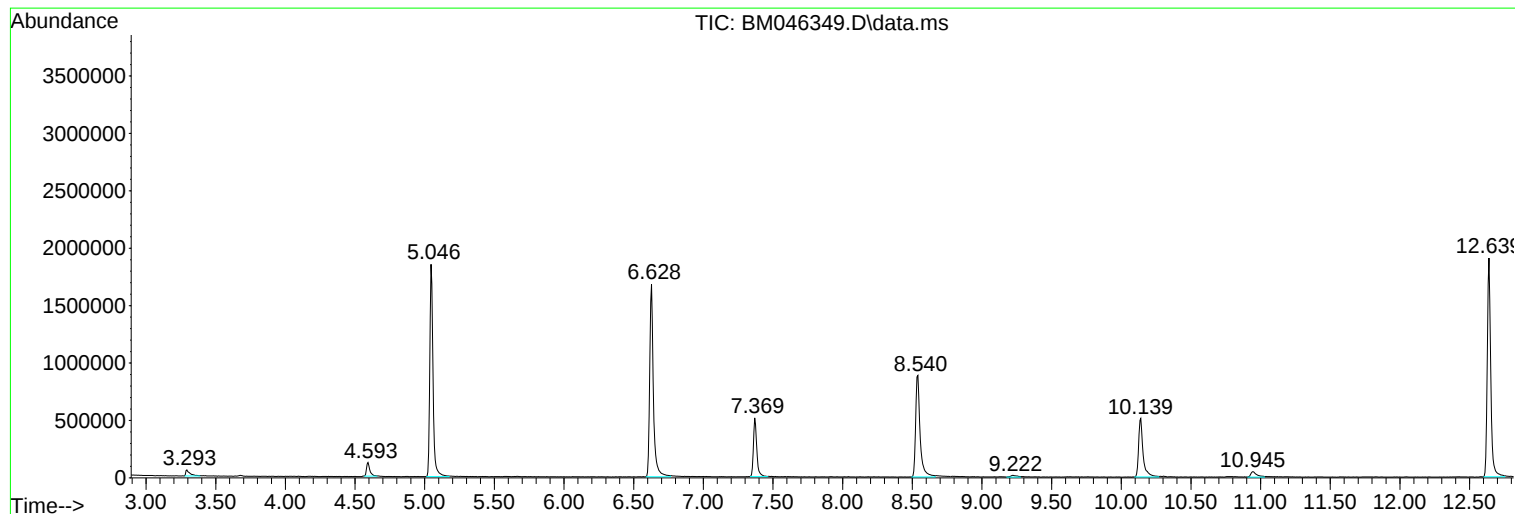
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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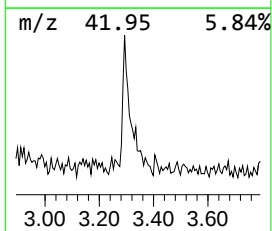
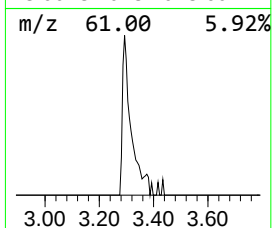
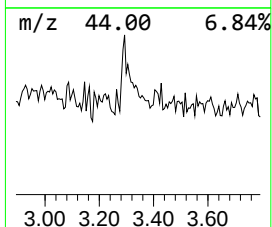
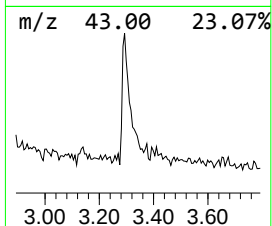
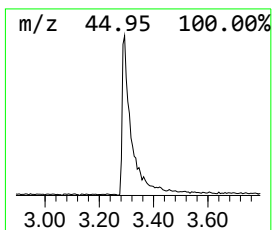
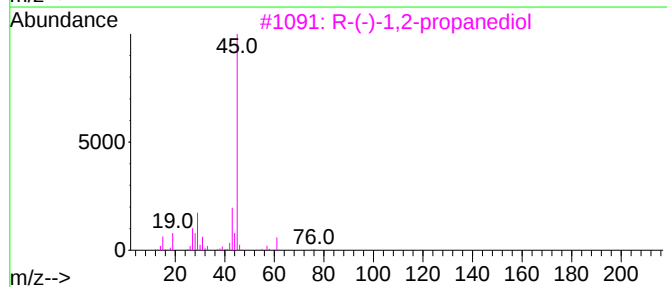
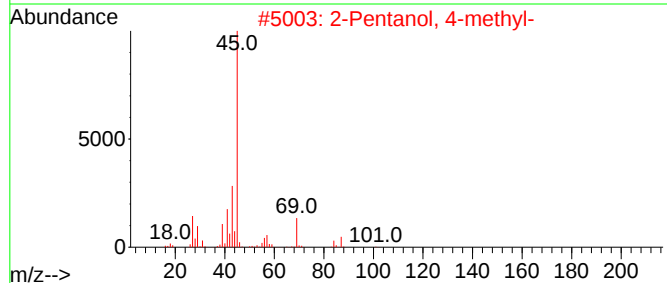
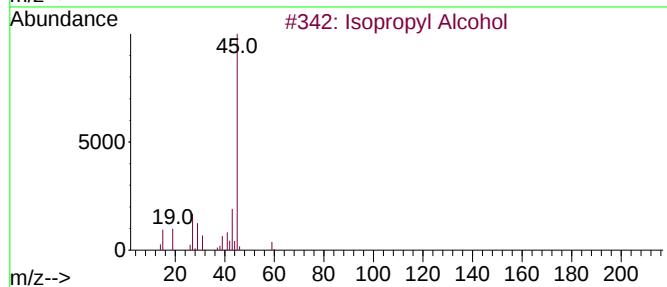
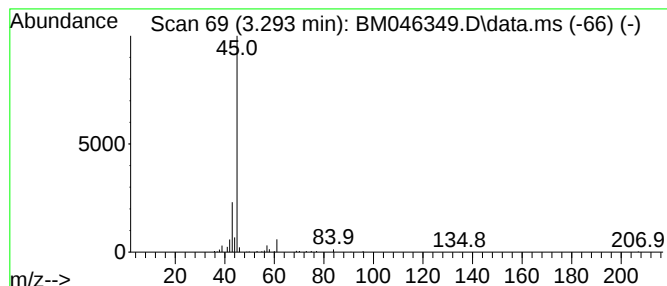
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.293	2.71 ng	116209	1,4-Dichlorobenzene-d4	7.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2			2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
4			Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	40
5			2-Heptanol, (S)-	116	C7H16O	006033-23-4	9



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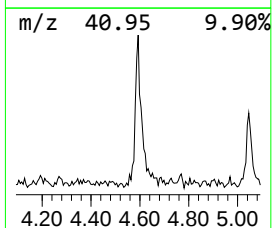
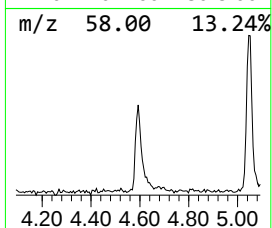
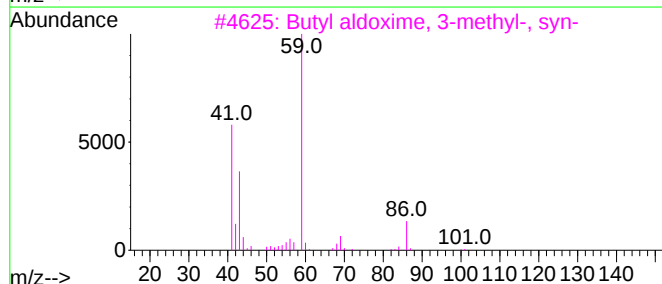
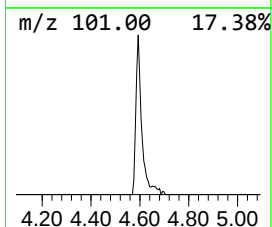
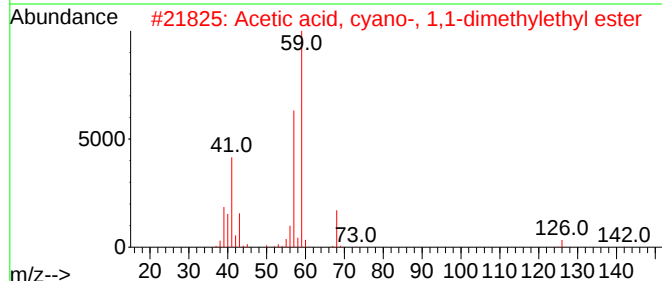
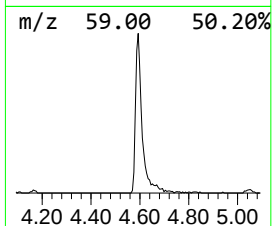
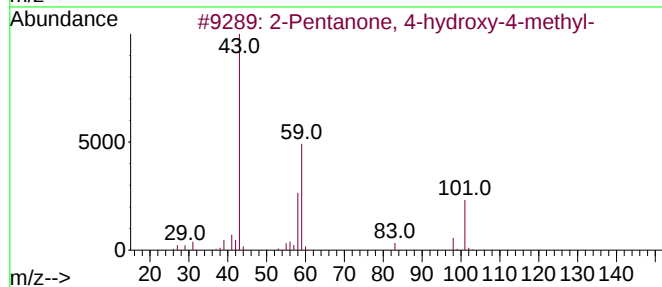
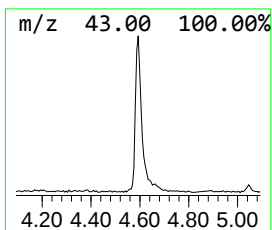
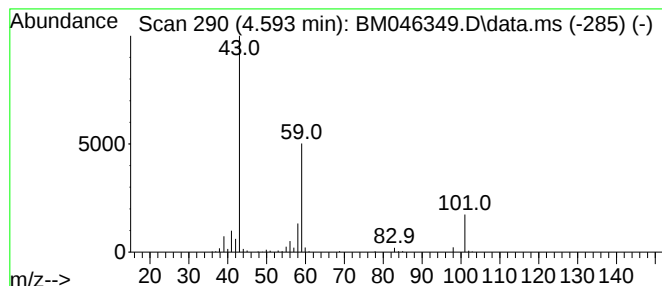
Instrument :
BNA_M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.593	4.60 ng	196878	1,4-Dichlorobenzene-d4			7.369
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	32
3	Butyl aldoxime, 3-methyl-, syn-		101	C5H11NO	005780-40-5	23
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9



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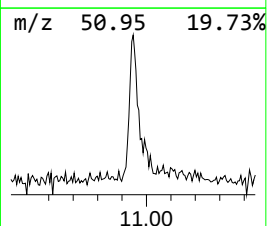
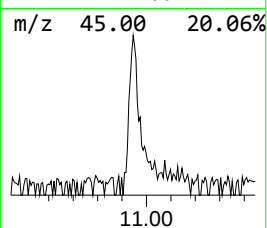
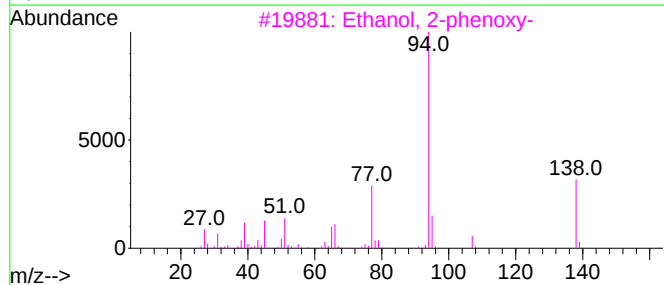
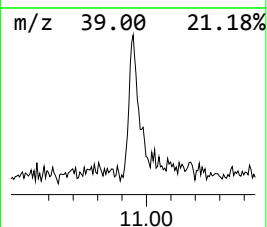
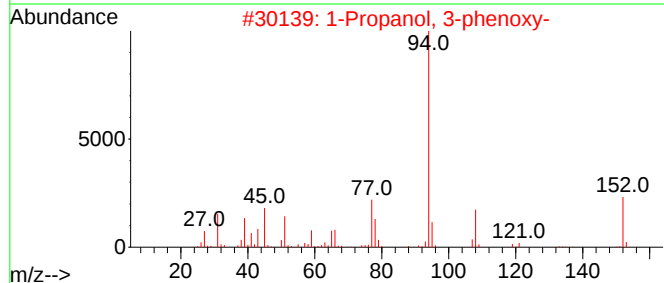
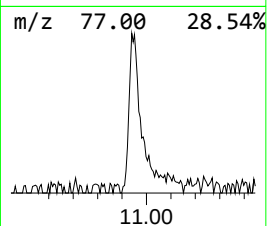
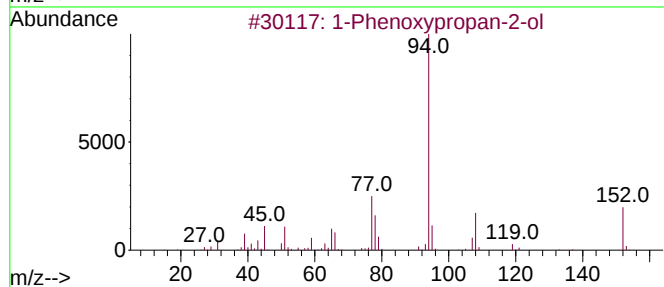
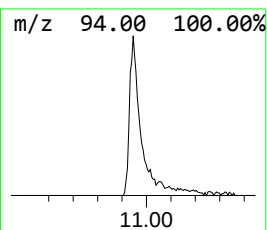
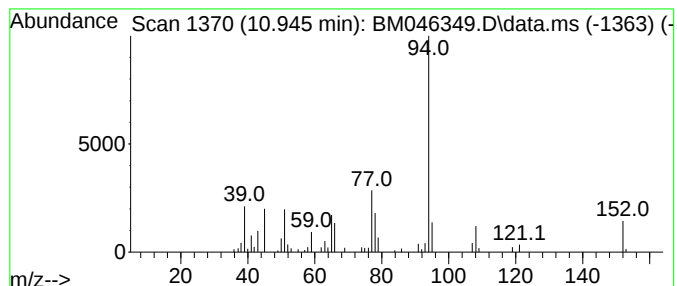
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Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	2.45 ng	136756	Naphthalene-d8	10.140

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	72
4			butanedioic acid, monophenyl ester	194	C10H10O4	1000400-29-4	50
5			2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	47



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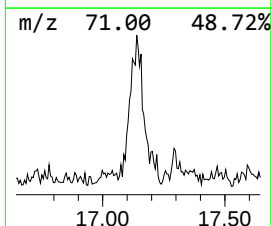
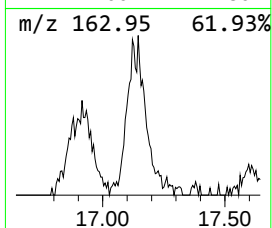
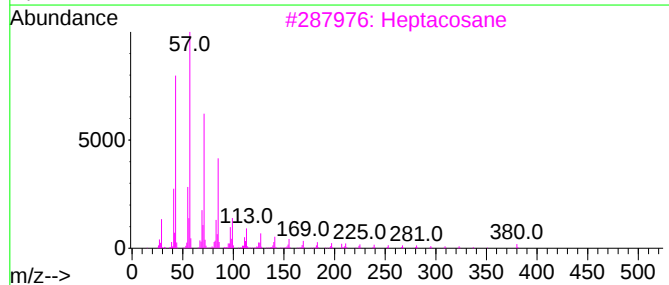
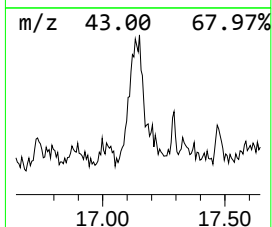
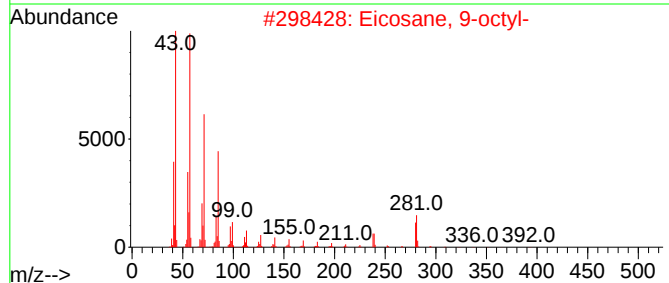
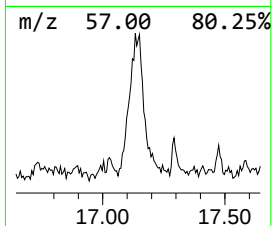
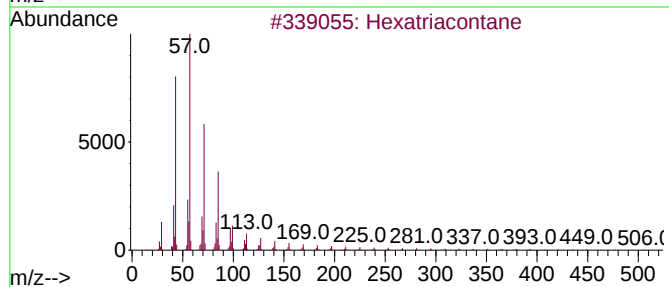
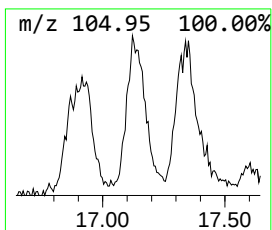
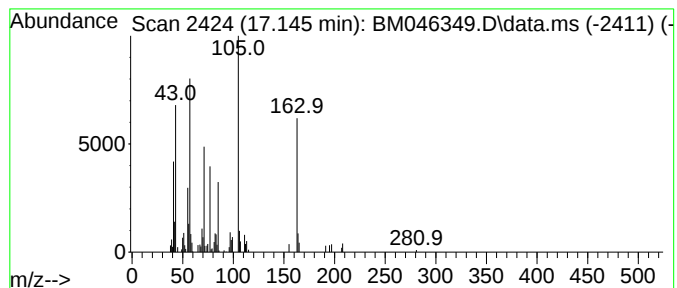
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Peak Number 4 unknown17.145 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.145	2.22 ng	168077	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontane	507	C36H74	000630-06-8	30
2			Eicosane, 9-octyl-	394	C28H58	013475-77-9	30
3			Heptacosane	380	C27H56	000593-49-7	30
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	30
5			Nonadecane	268	C19H40	000629-92-5	30



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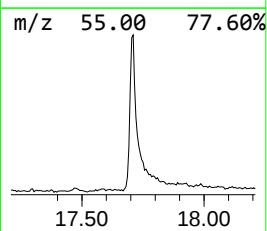
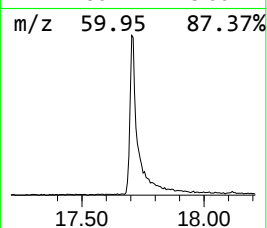
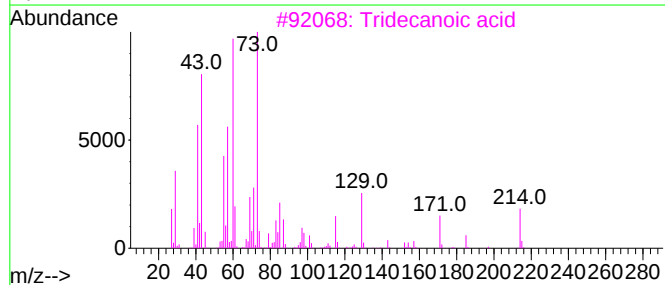
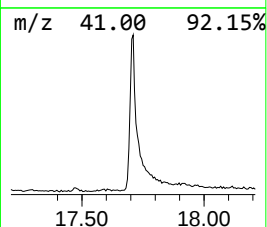
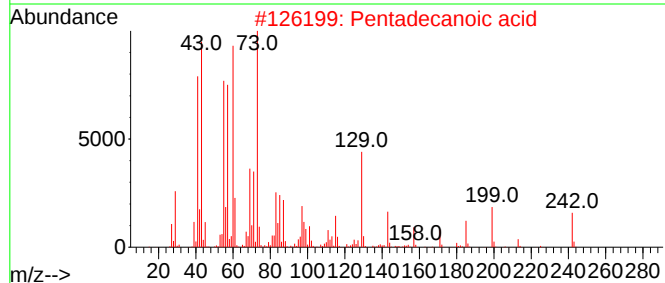
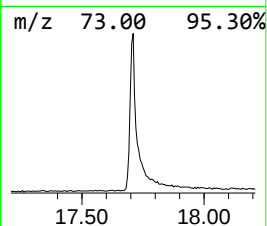
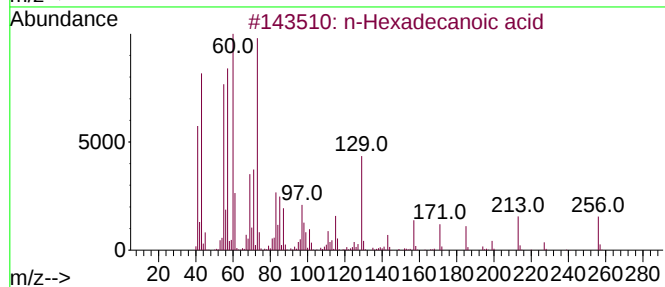
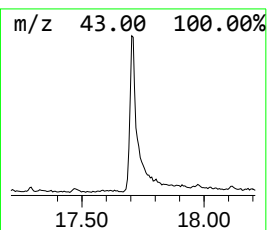
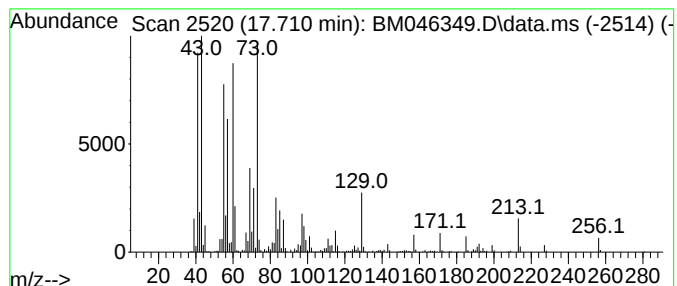
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.710	16.05 ng	1214510	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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ClientSampleId :
7-S-1

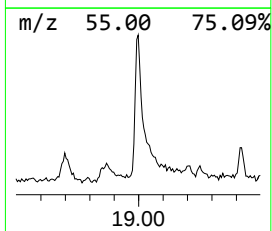
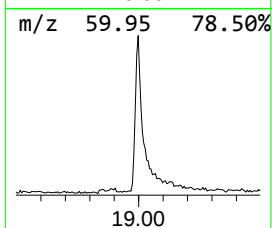
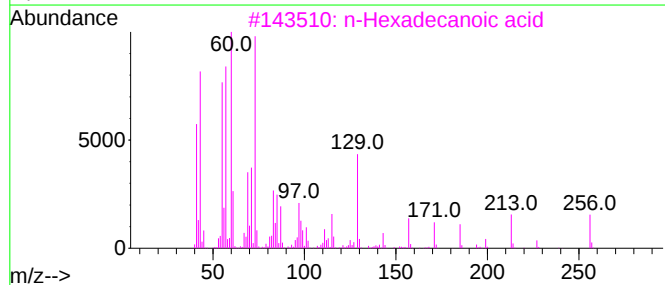
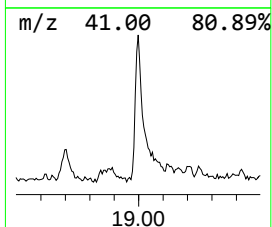
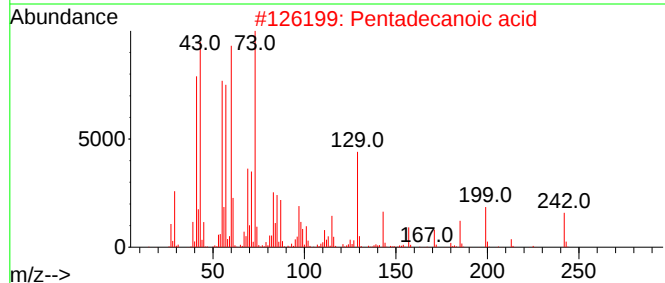
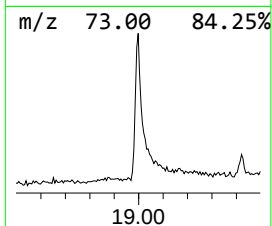
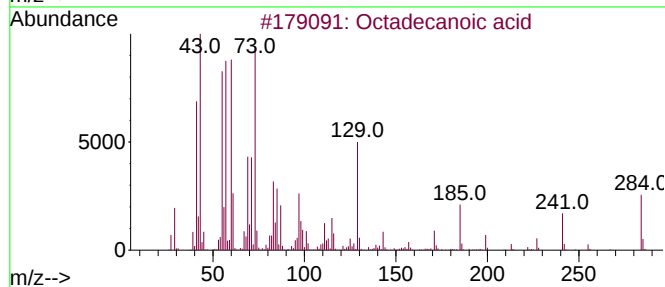
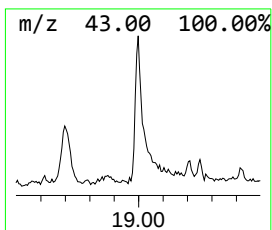
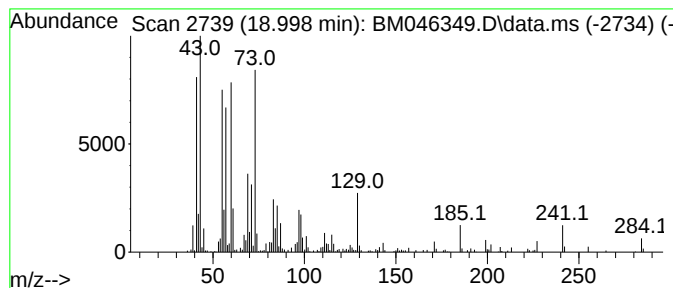
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.998	6.77 ng	511525	Chrysene-d12	20.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046349.D
Acq On : 28 Jun 2024 12:46
Operator : MA/JU
Sample : P3076-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

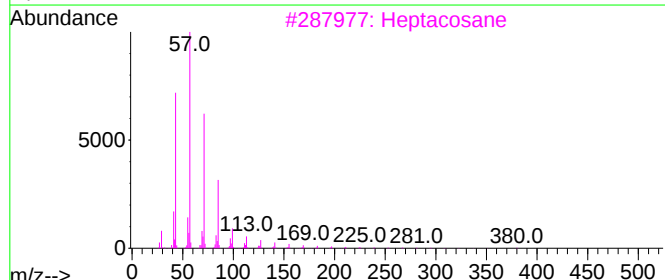
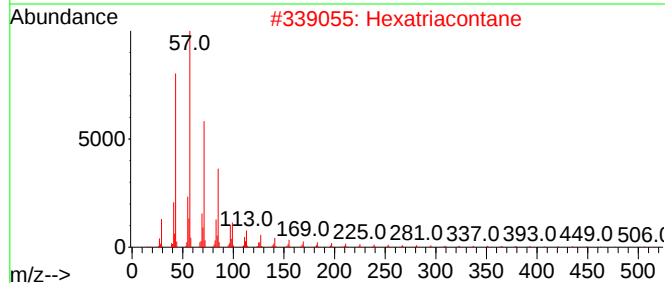
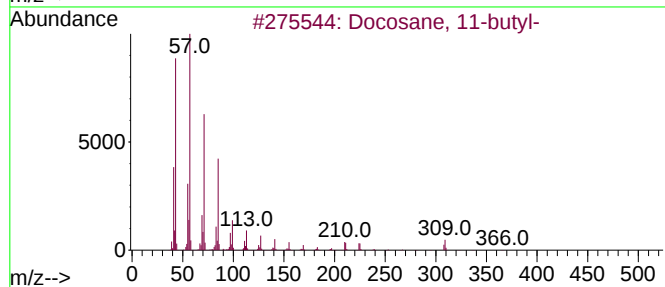
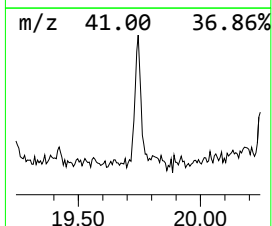
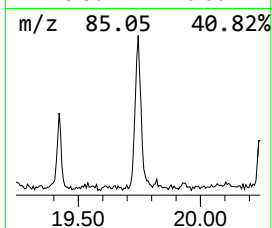
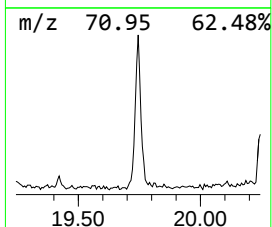
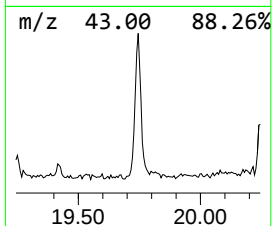
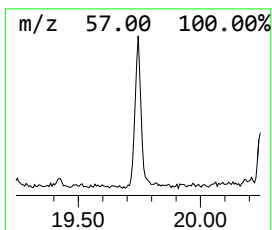
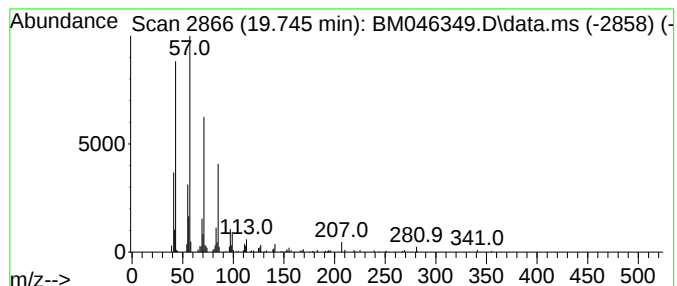
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosane, 11-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.745	3.01 ng	227429	Chrysene-d12		20.992	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-		366	C26H54	013475-76-8	90
2	Hexatriacontane		507	C36H74	000630-06-8	87
3	Heptacosane		380	C27H56	000593-49-7	87
4	Heneicosane		296	C21H44	000629-94-7	87
5	Tetracosane		338	C24H50	000646-31-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046349.D
Acq On : 28 Jun 2024 12:46
Operator : MA/JU
Sample : P3076-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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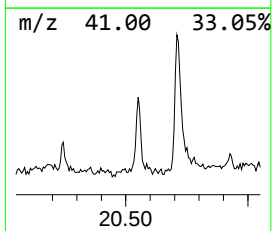
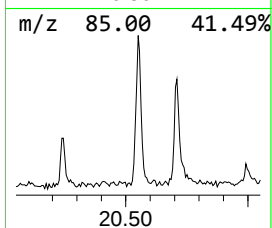
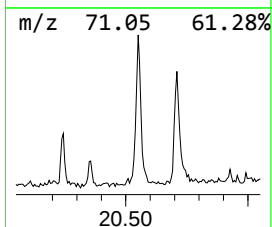
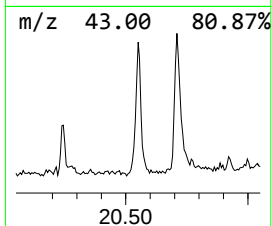
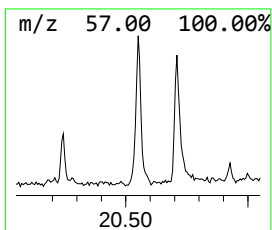
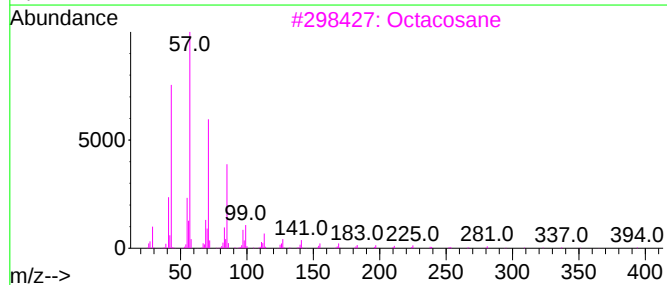
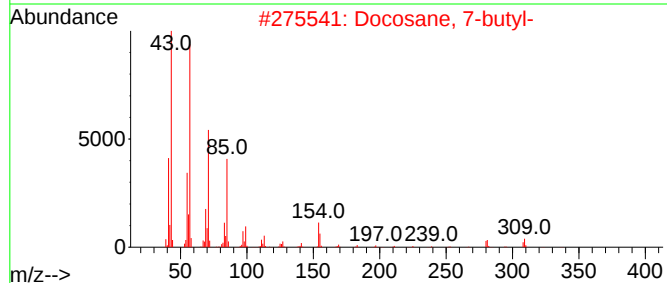
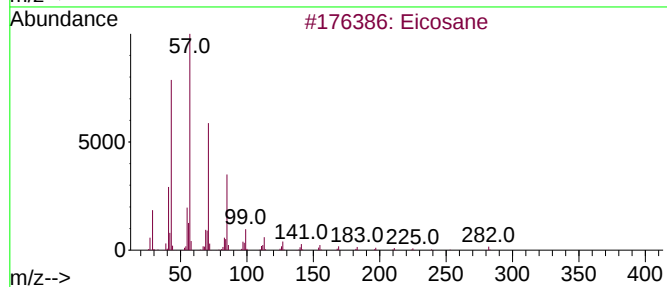
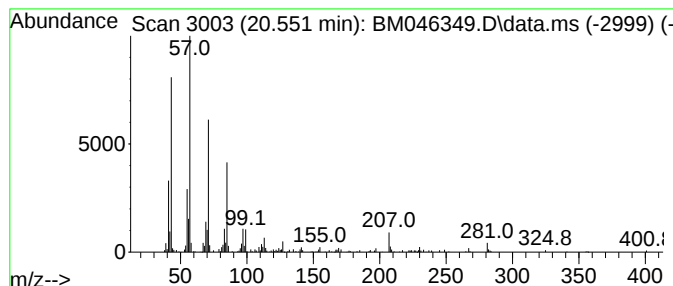
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.551	2.16 ng	163171	Chrysene-d12	20.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Docosane, 7-butyl-	366	C26H54	055282-15-0	83
3			Octacosane	394	C28H58	000630-02-4	83
4			Hexatriacontane	507	C36H74	000630-06-8	80
5			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046349.D
Acq On : 28 Jun 2024 12:46
Operator : MA/JU
Sample : P3076-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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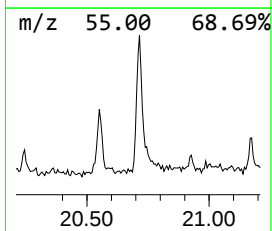
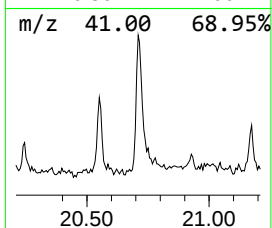
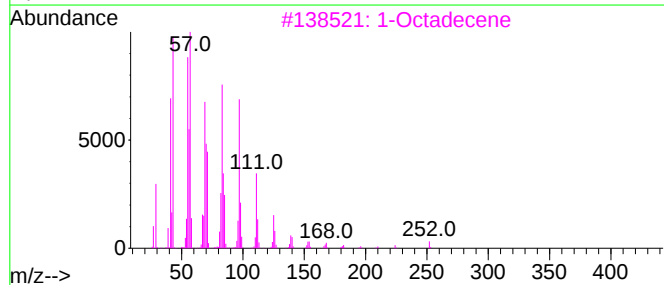
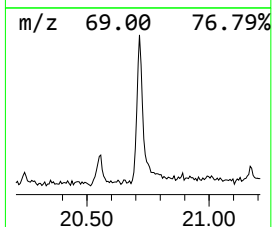
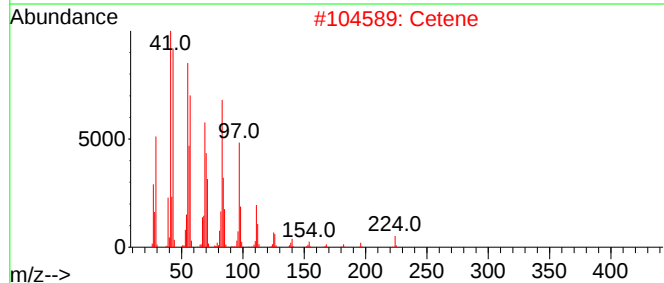
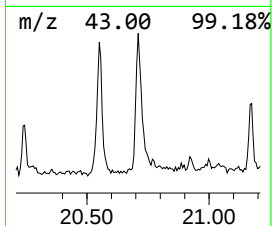
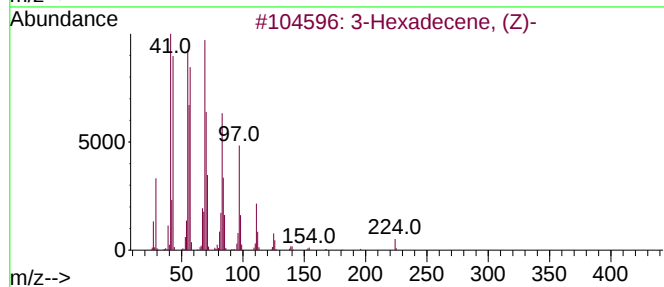
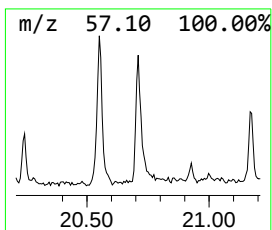
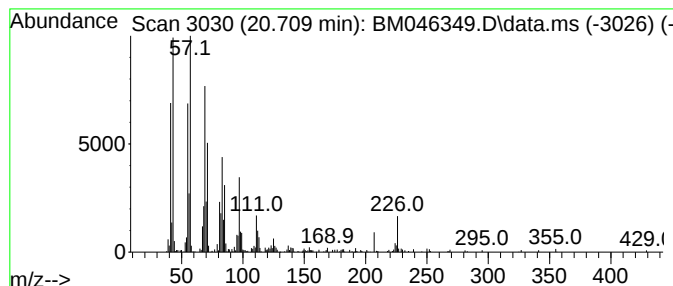
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3-Hexadecene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.709	4.88 ng	368902	Chrysene-d12	20.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexadecene, (Z)-	224	C16H32	034303-81-6	89
2			Cetene	224	C16H32	000629-73-2	80
3			1-Octadecene	252	C18H36	000112-88-9	64
4			Cyclohexadecane	224	C16H32	000295-65-8	59
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046349.D
Acq On : 28 Jun 2024 12:46
Operator : MA/JU
Sample : P3076-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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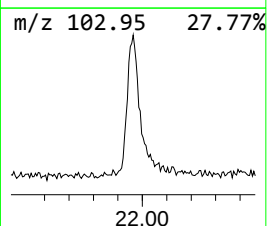
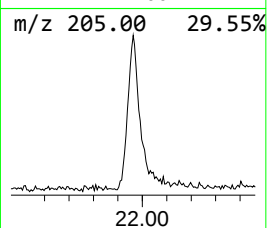
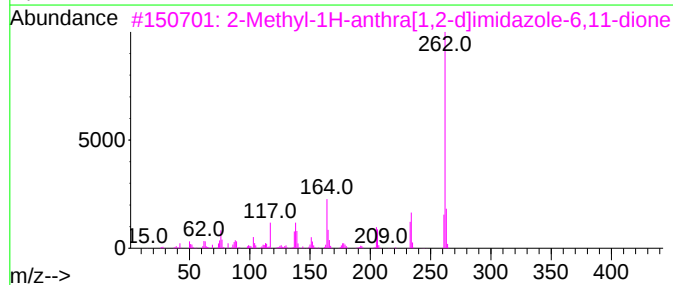
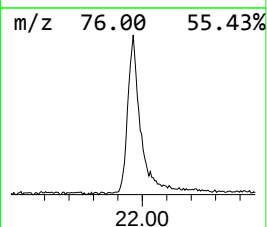
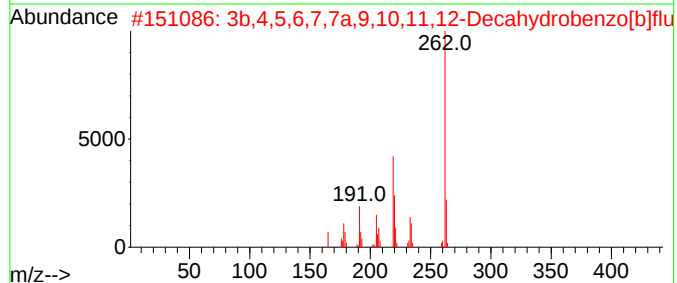
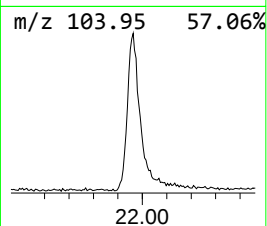
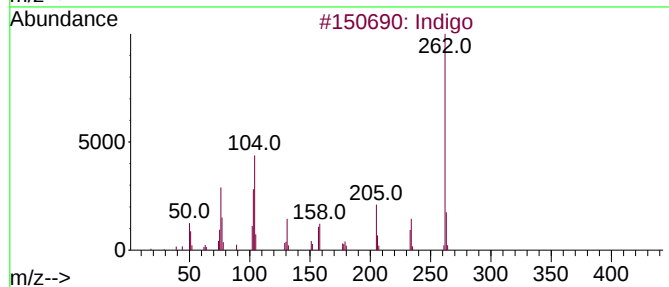
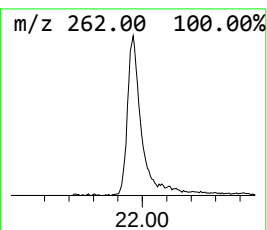
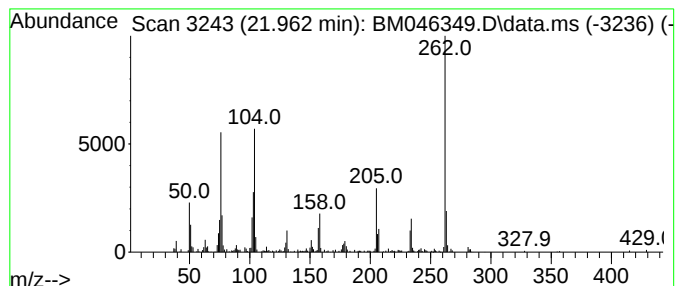
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Indigo Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.962	7.12 ng	537945	Chrysene-d12	20.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indigo	262	C16H10N2O2	000482-89-3	96
2			3b,4,5,6,7,7a,9,10,11,12-Decahyd...	262	C20H22	1000080-20-7	86
3			2-Methyl-1H-anthra[1,2-d]imidazo...	262	C16H10N2O2	030634-09-4	50
4			trans-Indigo	262	C16H10N2O2	064784-13-0	49
5			dibenzo[b,g][1,8]naphthyridine-1...	262	C16H10N2O2	1000396-82-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046349.D
Acq On : 28 Jun 2024 12:46
Operator : MA/JU
Sample : P3076-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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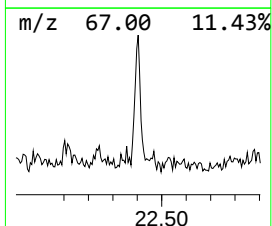
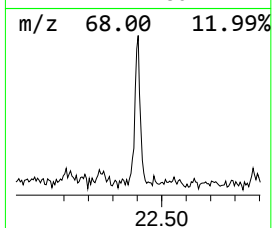
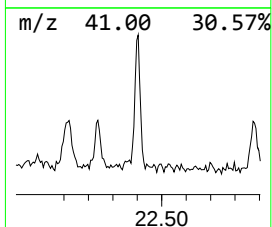
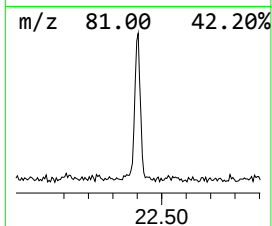
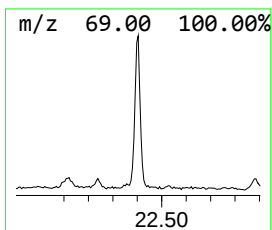
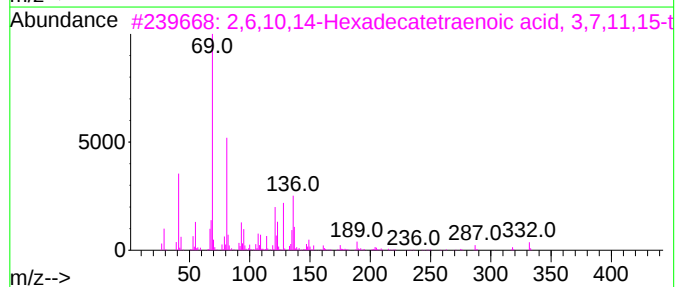
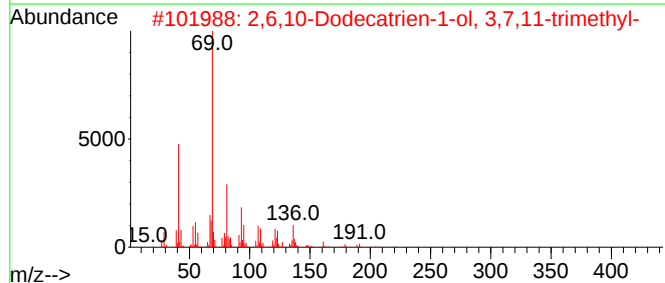
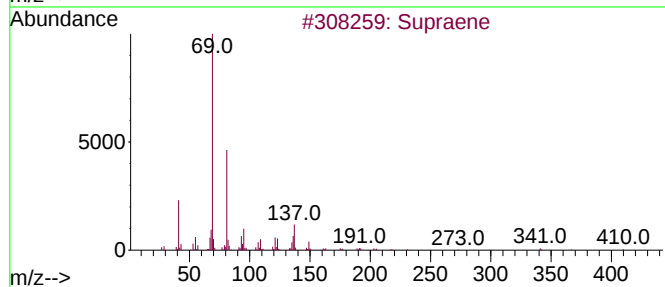
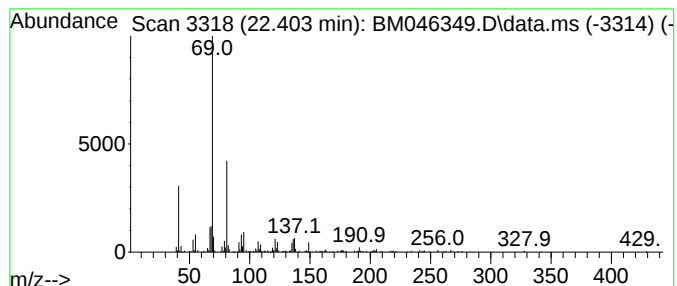
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.403	3.07 ng	212551	Perylene-d12	23.662

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	80
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
4			(2E,6E)-3,7,11-Trimethyldodeca-2...	376	C25H44O2	078368-57-7	72
5			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046349.D
Acq On : 28 Jun 2024 12:46
Operator : MA/JU
Sample : P3076-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

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

TIC Library : C:\Database\NIST0.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-...	4.593	4.6	ng	196878	1	7.369	856279	20.0
1-Phenoxypropan...	10.945	2.5	ng	136756	2	10.140	1114400	20.0
unknown17.145	17.145	2.2	ng	168077	4	16.774	1513070	20.0
n-Hexadecanoic ...	17.710	16.1	ng	1214510	4	16.774	1513070	20.0
Octadecanoic acid	18.998	6.8	ng	511525	5	20.992	1510880	20.0
Docosane, 11-bu...	19.745	3.0	ng	227429	5	20.992	1510880	20.0
Eicosane	20.551	2.2	ng	163171	5	20.992	1510880	20.0
3-Hexadecene, (Z)-	20.709	4.9	ng	368902	5	20.992	1510880	20.0
Indigo	21.962	7.1	ng	537945	5	20.992	1510880	20.0
Supraene	22.403	3.1	ng	212551	6	23.662	1383040	20.0