

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
 Data File : BF138744.D
 Acq On : 02 Aug 2024 13:30
 Operator : RC/JU
 Sample : P3402-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 355

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_F\Methods\8270-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138744.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	14	rVB	1072380	1289630	70.77%	8.057%
2	3.363	211	216	238	rBV	19918	65841	3.61%	0.411%
3	5.063	500	505	520	rVB	77075	115616	6.34%	0.722%
4	5.469	569	574	597	rBV	1137190	1506582	82.68%	9.413%
5	6.481	740	746	762	rBV	1194269	1583160	86.88%	9.891%
6	6.845	803	808	813	rBV	354442	449685	24.68%	2.809%
7	7.404	897	903	908	rBV	792146	1037923	56.96%	6.485%
8	7.657	941	946	952	rBV	26005	33385	1.83%	0.209%
9	8.122	1020	1025	1036	rBV	483002	610927	33.53%	3.817%
10	8.433	1074	1078	1093	rBV	58278	93011	5.10%	0.581%
11	9.198	1202	1208	1213	rBV	1489457	1822293	100.00%	11.385%
12	9.298	1217	1225	1233	rVB	155962	194511	10.67%	1.215%
13	9.875	1318	1323	1333	rVB	520958	659800	36.21%	4.122%
14	9.975	1333	1340	1352	rBV	631236	1014412	55.67%	6.338%
15	10.080	1354	1358	1363	rVB	16601	20827	1.14%	0.130%
16	10.669	1452	1458	1466	rBV	694932	929495	51.01%	5.807%
17	11.363	1571	1576	1591	rVB	476059	641916	35.23%	4.010%
18	11.892	1658	1666	1677	rBV3	54324	104693	5.75%	0.654%
19	12.451	1752	1761	1768	rBV6	22980	51478	2.82%	0.322%
20	12.574	1778	1782	1791	rVB	41310	62631	3.44%	0.391%
21	12.674	1795	1799	1803	rBV3	12544	21436	1.18%	0.134%
22	12.810	1816	1822	1825	rBV3	37012	56329	3.09%	0.352%
23	12.945	1840	1845	1850	rBV	1108331	1396443	76.63%	8.725%
24	13.168	1879	1883	1887	rBV	28267	39525	2.17%	0.247%
25	13.374	1913	1918	1921	rBV	57779	82928	4.55%	0.518%
26	13.410	1921	1924	1934	rVB4	48154	83725	4.59%	0.523%
27	13.510	1937	1941	1945	rBV2	26521	38206	2.10%	0.239%
28	13.851	1993	1999	2015	rVV3	73719	192005	10.54%	1.200%
29	14.004	2016	2025	2035	rVB	298872	445871	24.47%	2.786%
30	14.157	2047	2051	2056	rBV	22516	31390	1.72%	0.196%
31	14.462	2099	2103	2105	rBV	26590	36538	2.01%	0.228%
32	14.498	2106	2109	2114	rVB	23582	40622	2.23%	0.254%
33	14.621	2126	2130	2135	rBV	78020	117979	6.47%	0.737%
34	14.757	2149	2153	2158	rVB2	54603	107075	5.88%	0.669%
35	15.039	2198	2201	2207	rBV	16476	24827	1.36%	0.155%
36	15.098	2207	2211	2216	rVB	38058	53832	2.95%	0.336%

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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 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_F\Methods\8270-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.157	2216	2221	2234	rBV7	28568	94542	5.19%	0.591%
38	15.468	2267	2274	2286	rBV	267505	439131	24.10%	2.744%
39	15.680	2306	2310	2317	rBV5	17263	26494	1.45%	0.166%
40	15.909	2343	2349	2354	rBV	52021	87401	4.80%	0.546%
41	16.004	2357	2365	2367	rBV7	21788	57427	3.15%	0.359%
42	16.574	2459	2462	2474	rVB7	12415	26247	1.44%	0.164%
43	16.704	2480	2484	2491	rVB7	13315	24158	1.33%	0.151%
44	16.998	2528	2534	2543	rVB	33234	75892	4.16%	0.474%
45	17.533	2618	2625	2637	rBV	16277	62116	3.41%	0.388%
46	18.515	2785	2792	2801	rVB6	19306	56006	3.07%	0.350%

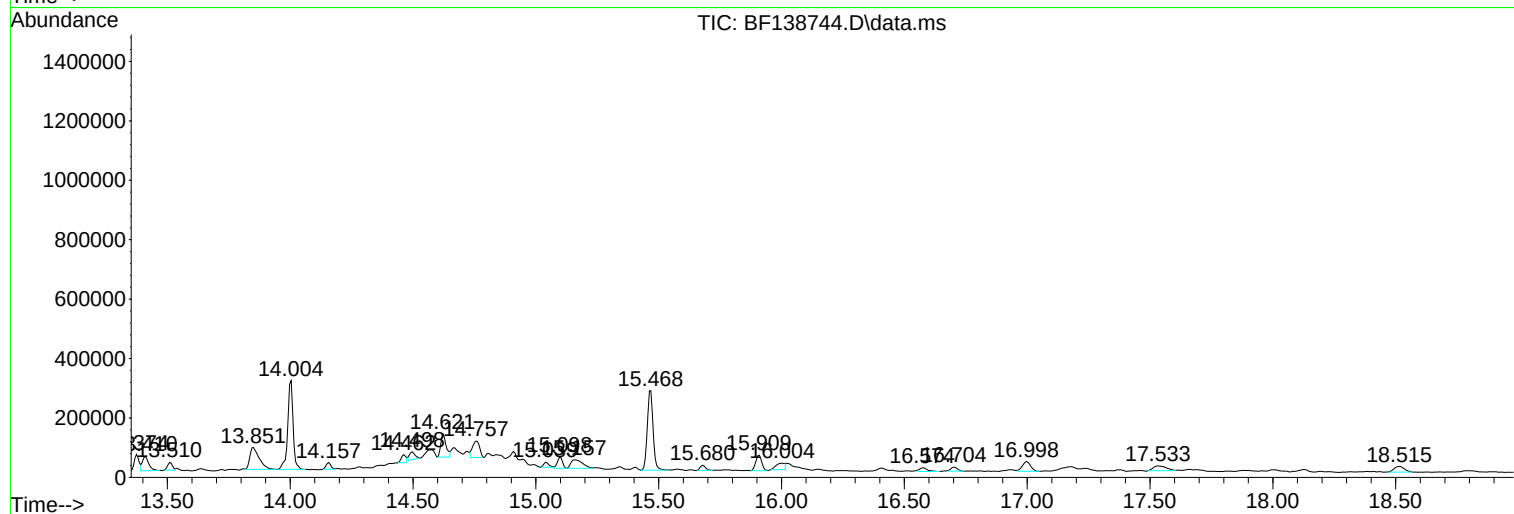
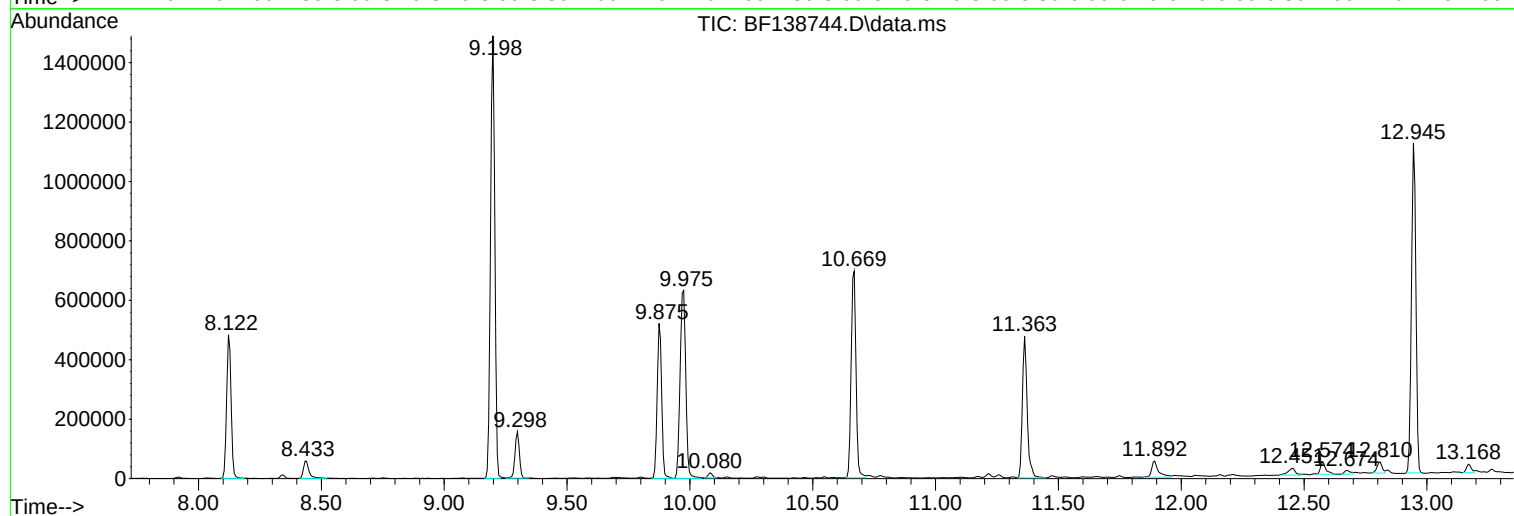
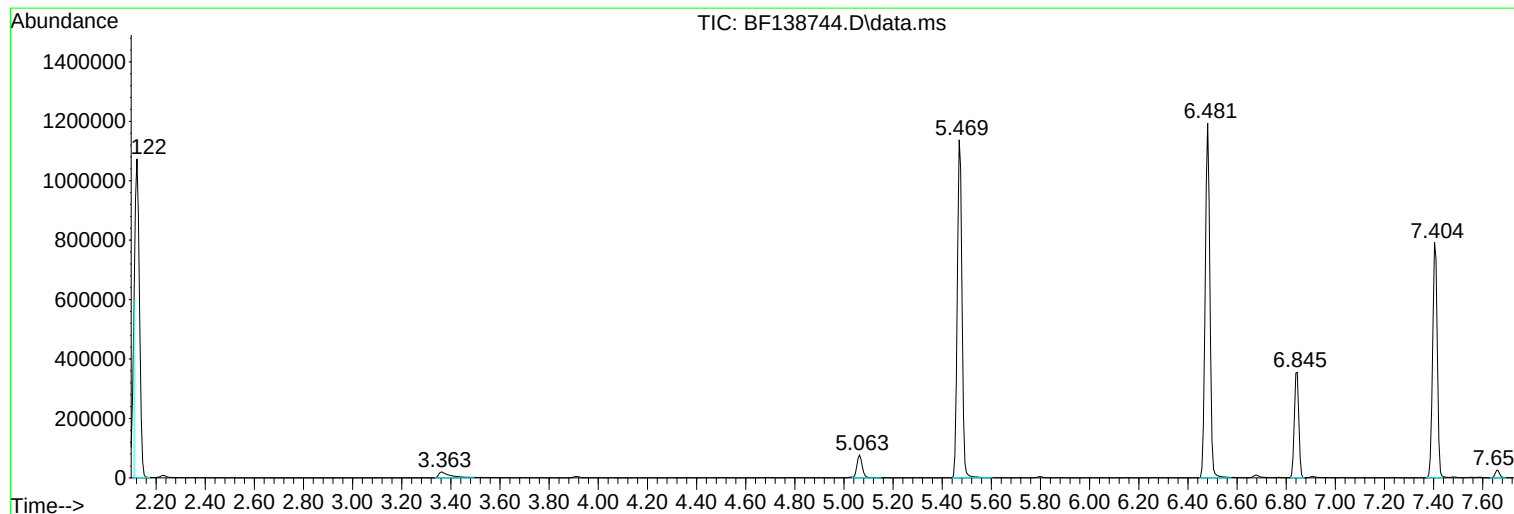
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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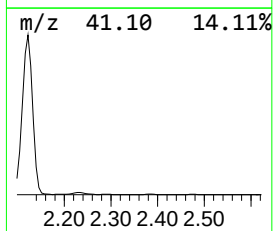
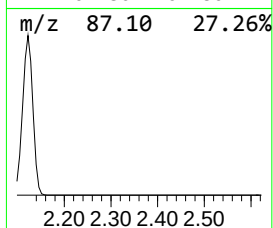
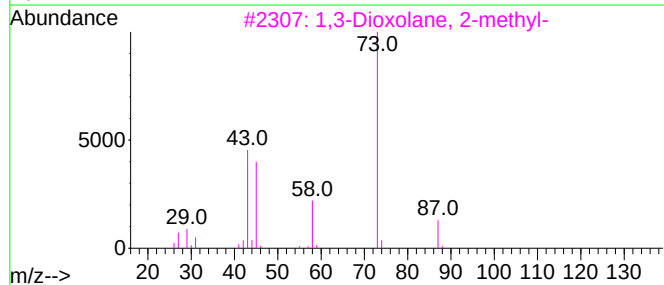
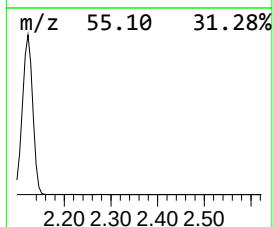
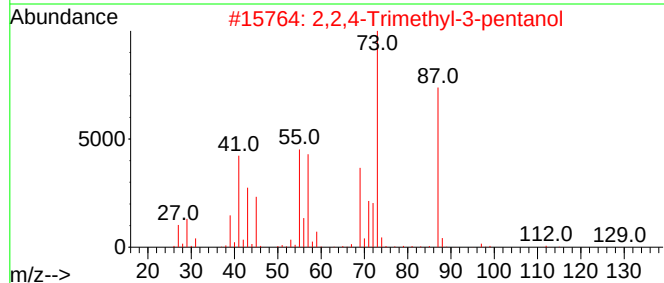
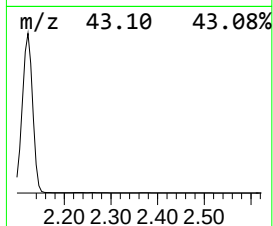
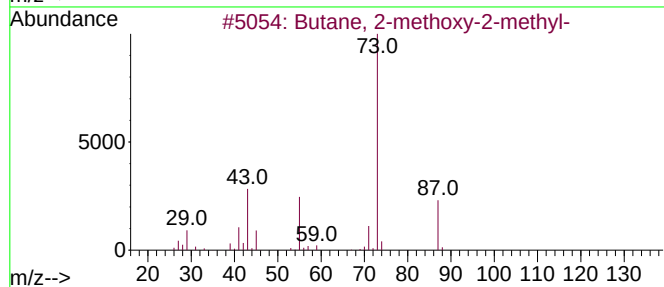
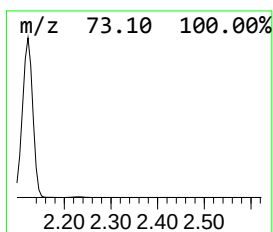
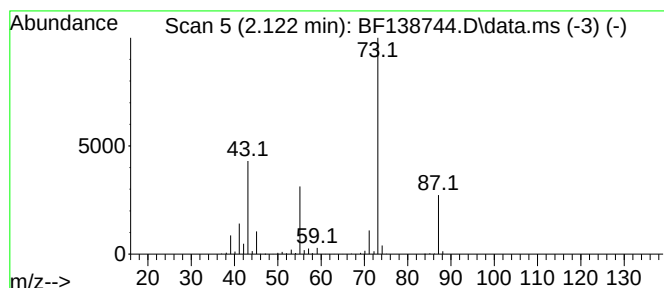
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	57.36 ng	1289630	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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Misc :
ALS Vial : 10 Sample Multiplier: 1

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BNA_F
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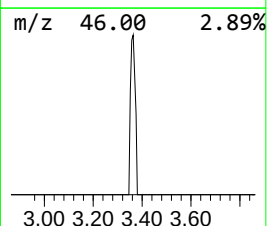
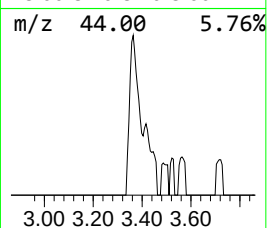
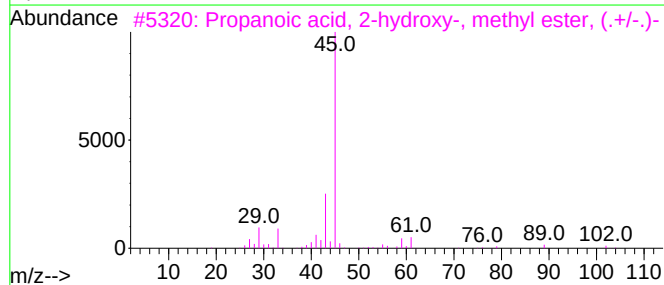
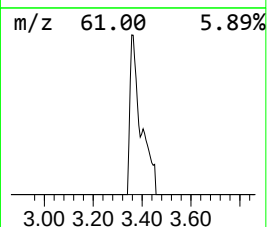
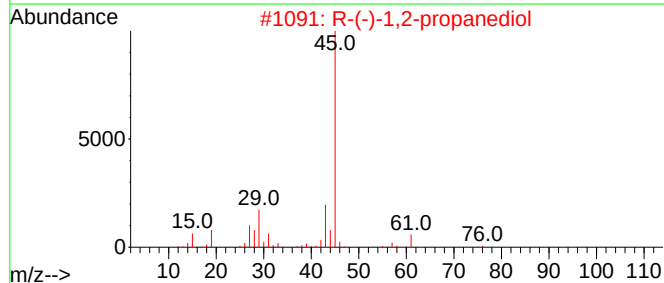
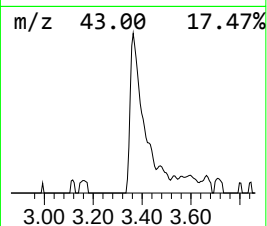
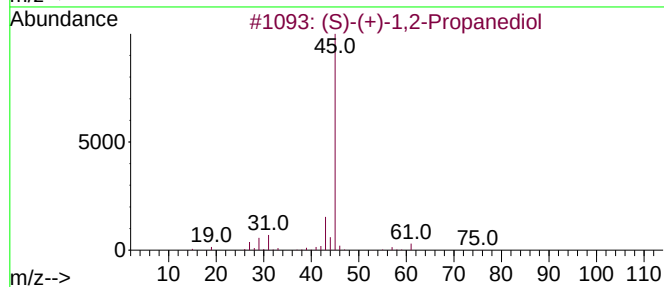
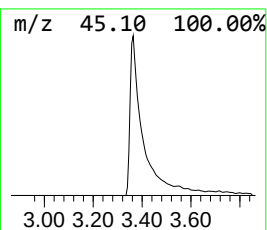
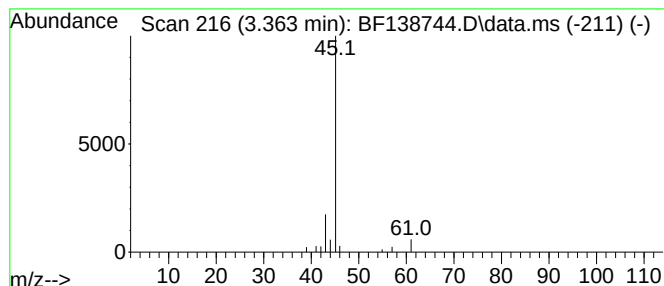
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	2.93 ng	65841	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	74
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	64
3	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	9
4	Propylene Glycol			76	C3H8O2	000057-55-6	9
5	Formamide			45	CH3NO	000075-12-7	7



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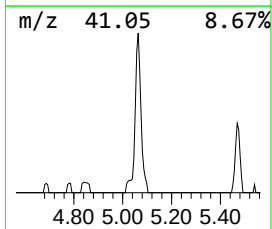
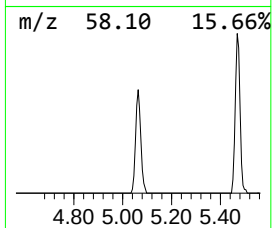
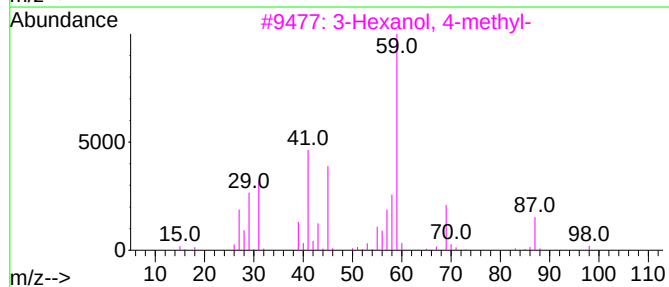
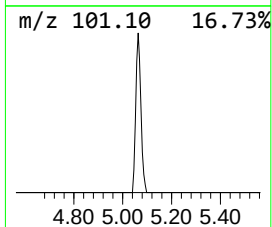
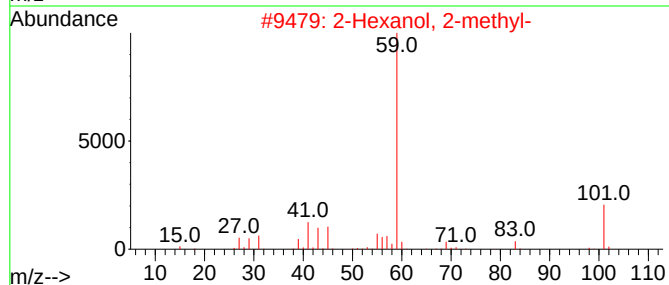
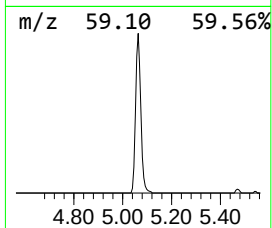
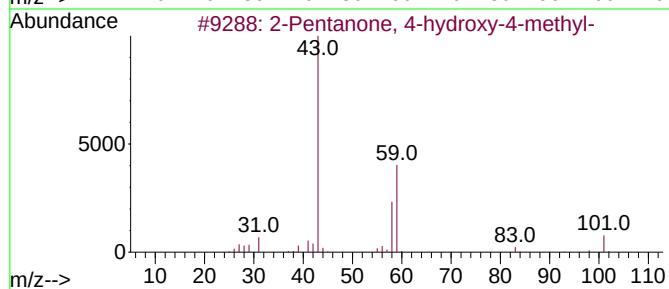
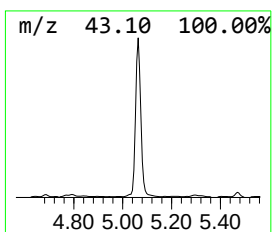
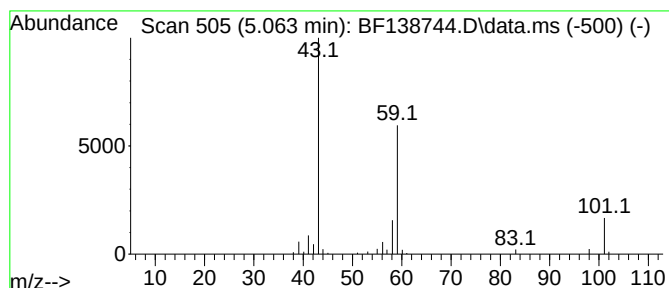
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	5.14 ng	115616	1,4-Dichlorobenzene-d4	6.845

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	



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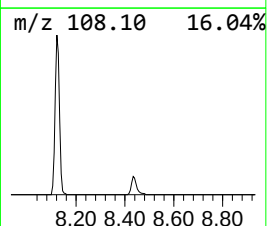
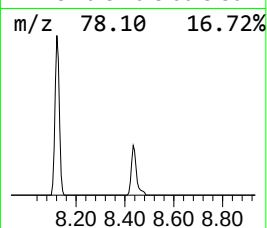
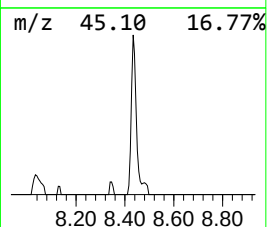
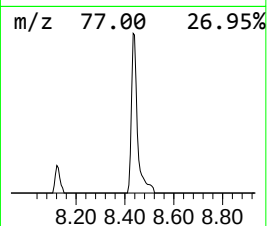
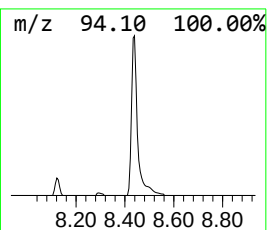
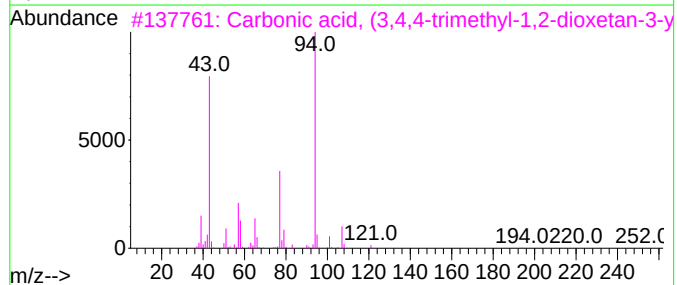
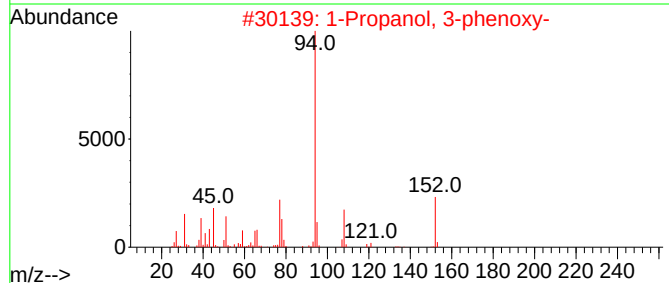
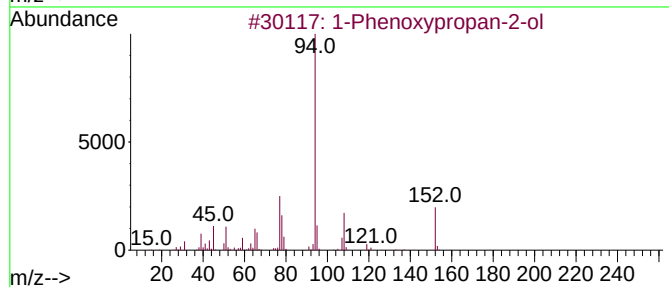
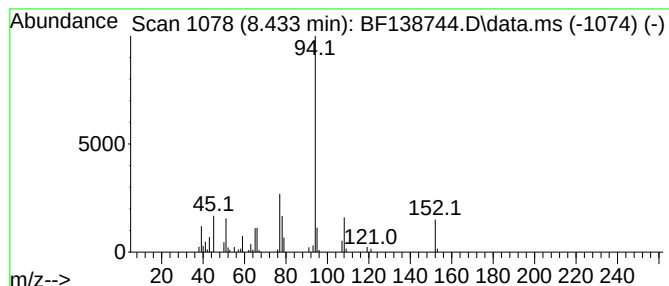
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	3.04 ng	93011	Naphthalene-d8	8.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3			Carbonic acid, (3,4,4-trimethyl-...	252	C13H16O5	109123-69-5	59
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59



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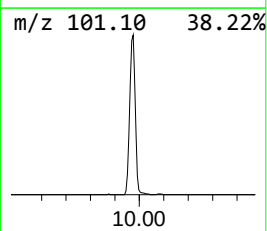
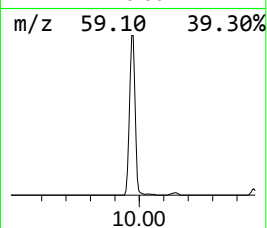
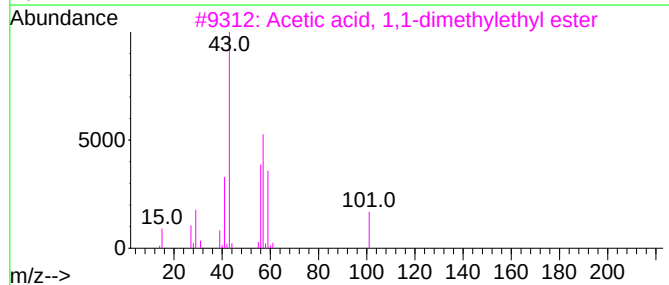
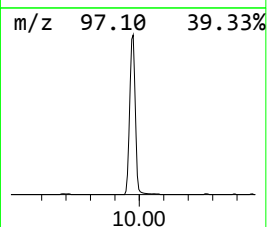
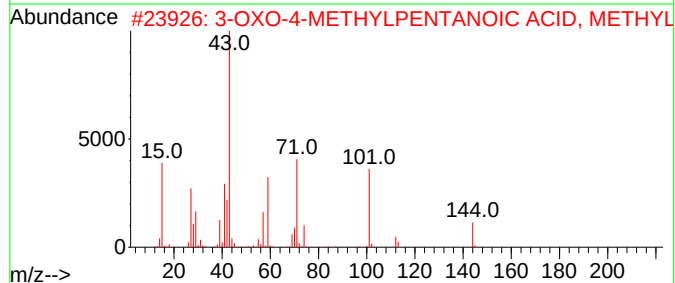
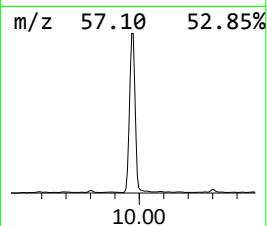
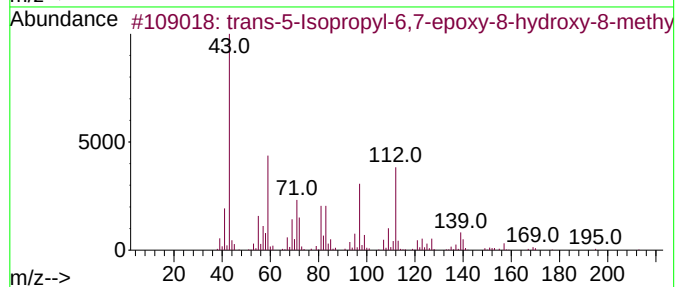
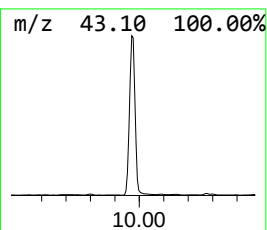
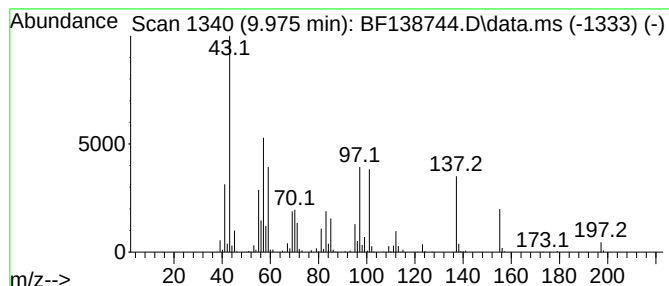
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.975 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.975	30.75 ng	1014410	Acenaphthene-d10	9.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	25
2			3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12
4			11-Tricosene	322	C23H46	052078-56-5	12
5			3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
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Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

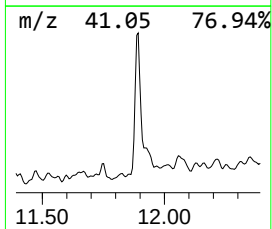
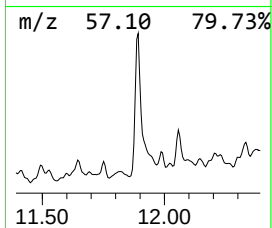
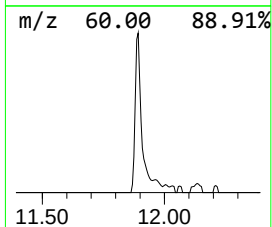
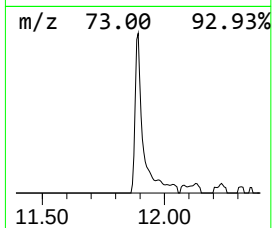
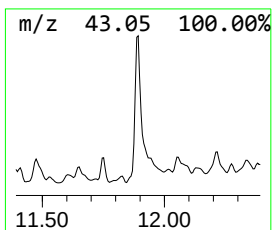
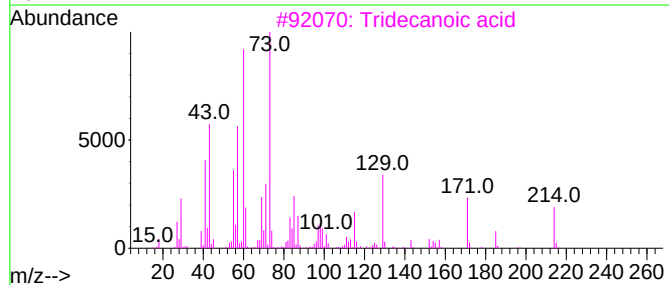
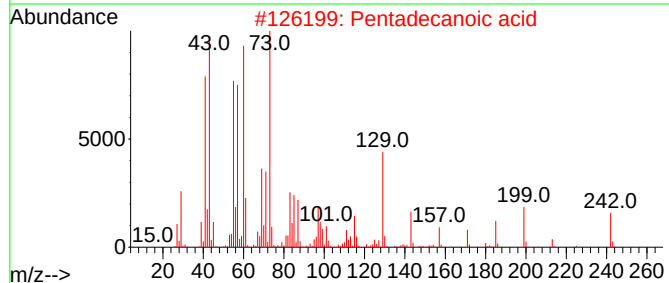
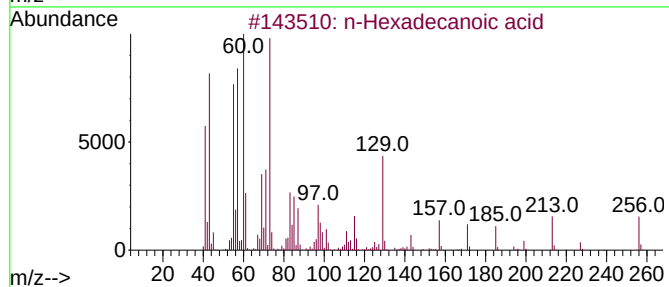
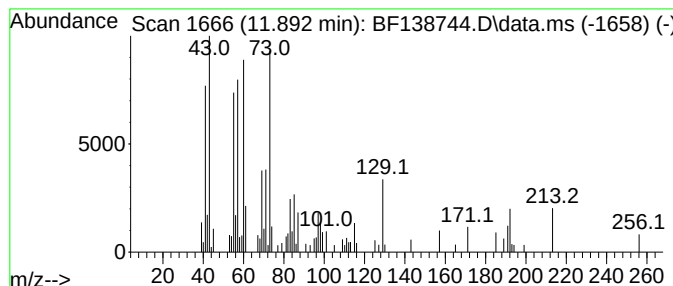
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.892	3.26 ng	104693	Phenanthrene-d10	11.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Butyl n-pentyl disulfide	192	C9H20S2	072437-52-6	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
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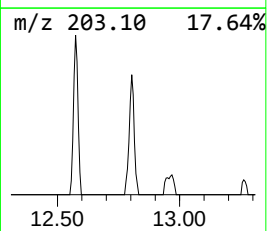
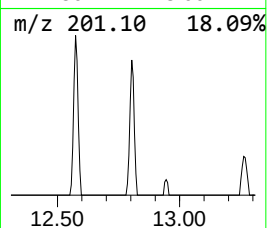
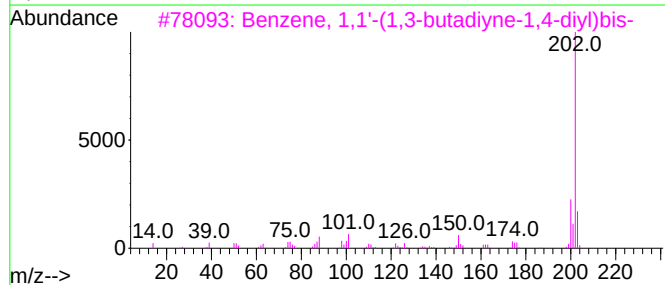
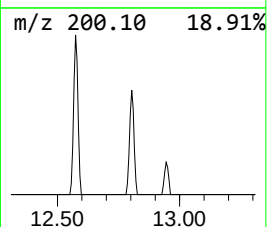
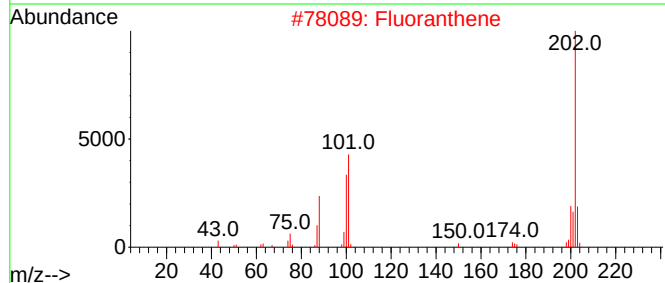
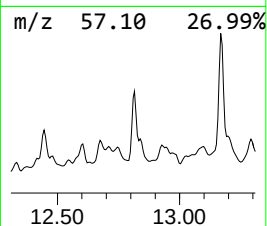
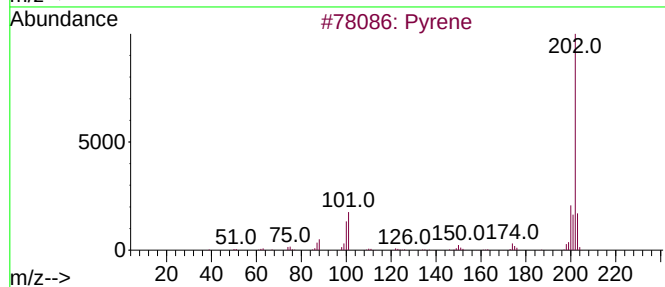
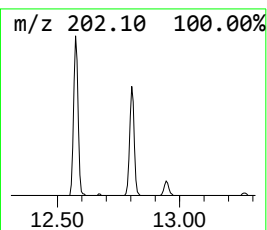
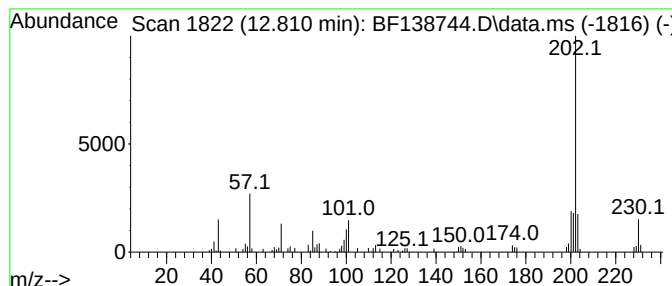
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.810	2.53 ng	56329	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene	202	C16H10	000129-00-0	95
2			Fluoranthene	202	C16H10	000206-44-0	81
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
4			1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	59
5			8-Methoxy-2-[n-propyl]-5,6-dihyd...	230	C14H18N2O	059353-29-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
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Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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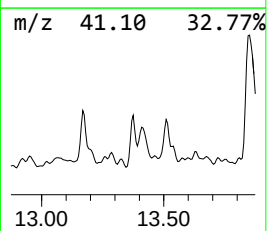
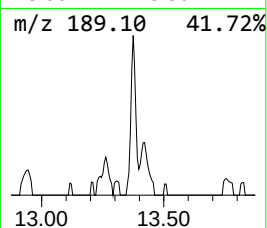
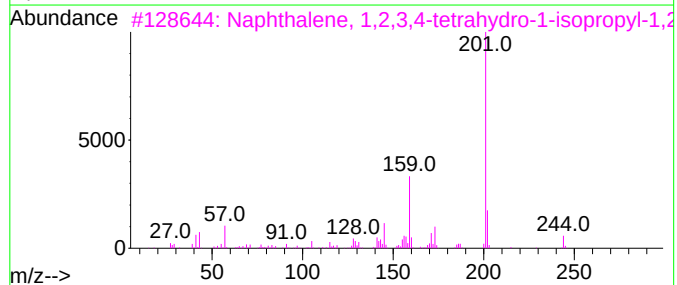
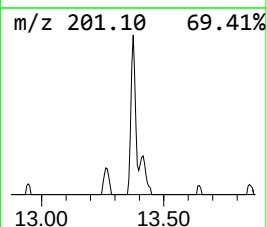
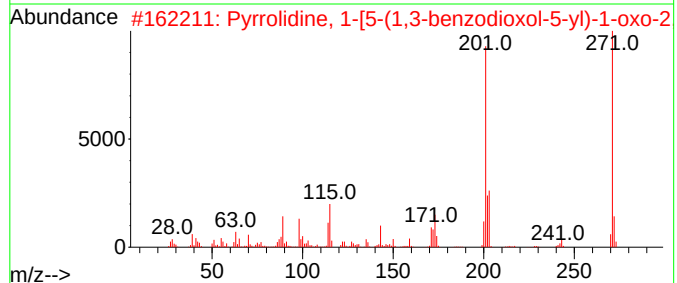
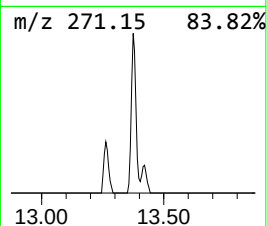
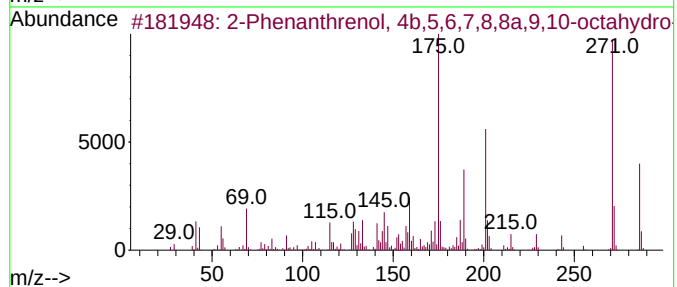
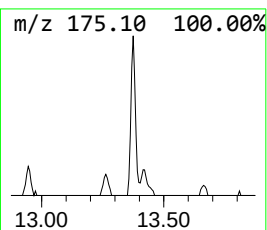
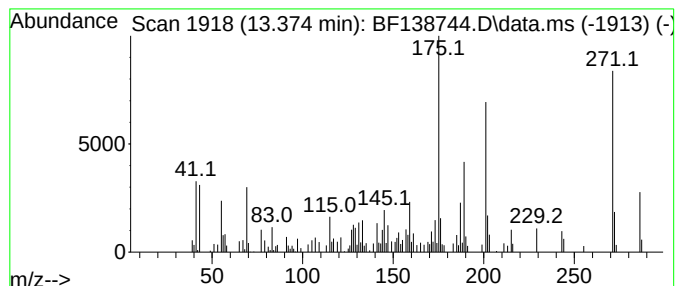
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.374	3.72 ng	82928	Chrysene-d12	14.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2		Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	38
3		Naphthalene, 1,2,3,4-tetrahydro-...	244	C18H28	029577-17-1	25
4		Crinan-1-one	271	C16H17NO3	098301-98-5	20
5		(-)-Morphinan-6-one, 4-methoxy-	271	C17H21NO2	1000129-09-1	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
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Acq On : 02 Aug 2024 13:30
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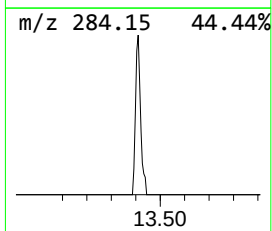
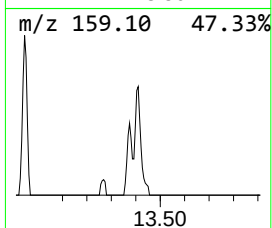
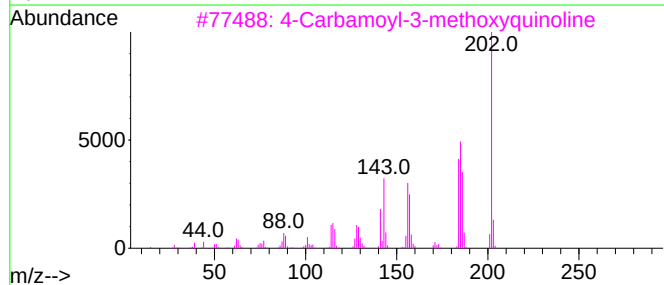
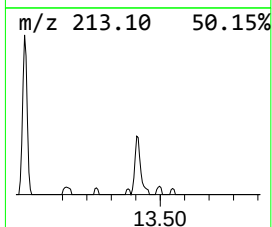
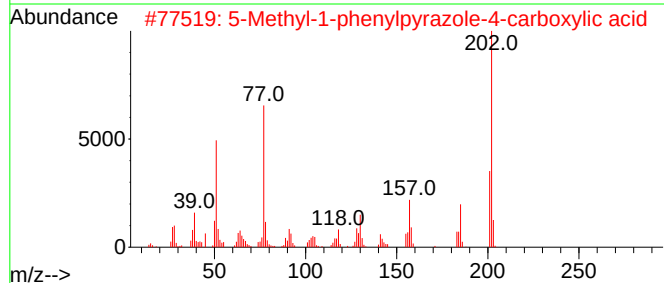
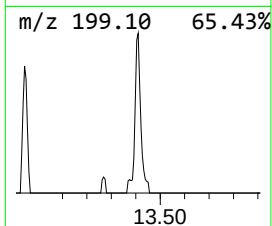
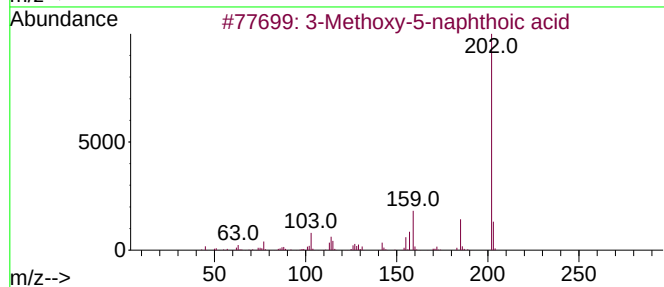
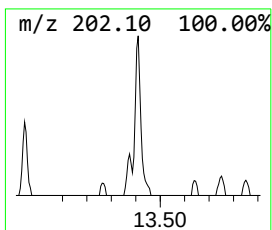
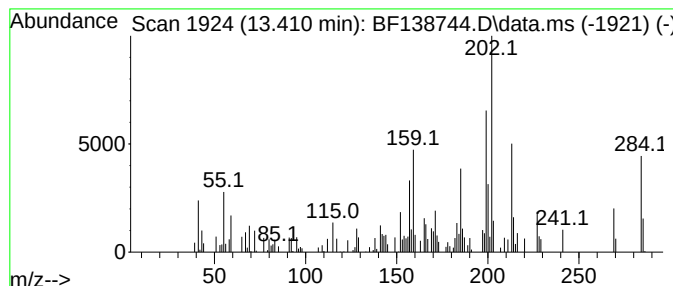
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.410 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.410	3.76 ng	83725	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methoxy-5-naphthoic acid	202	C12H10O3	007498-58-0	35
2			5-Methyl-1-phenylpyrazole-4-carb...	202	C11H10N2O2	091138-00-0	35
3			4-Carbamoyl-3-methoxyquinoline	202	C11H10N2O2	020844-05-7	30
4			1-Naphthalenecarboxylic acid, 2-...	202	C12H10O3	000947-62-6	25
5			8-Amino-2,5-dimethyl-6-methoxyqu...	202	C12H14N2O	1000214-69-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
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ALS Vial : 10 Sample Multiplier: 1

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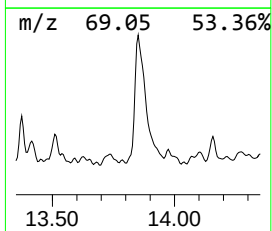
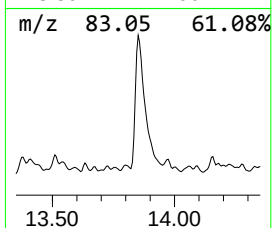
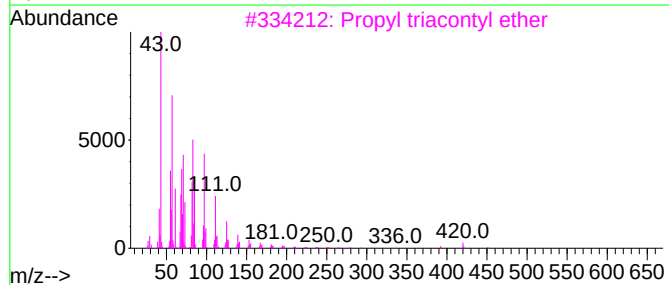
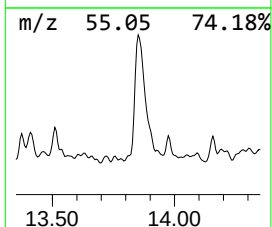
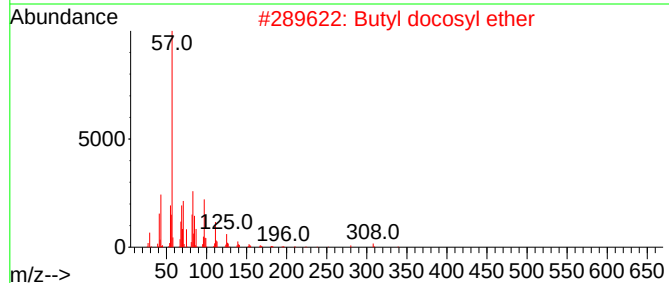
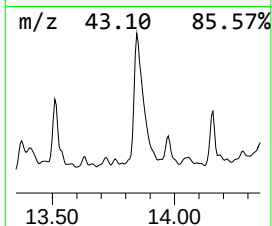
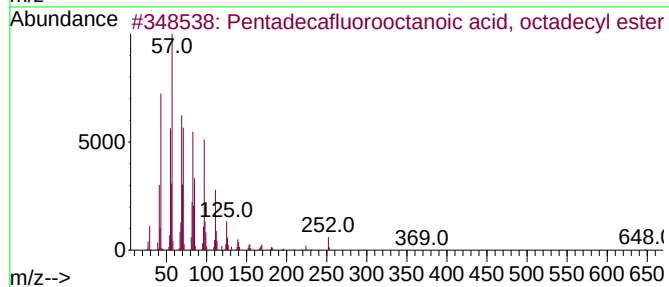
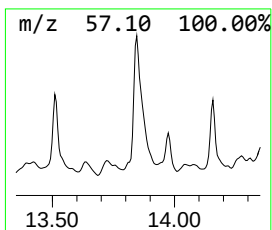
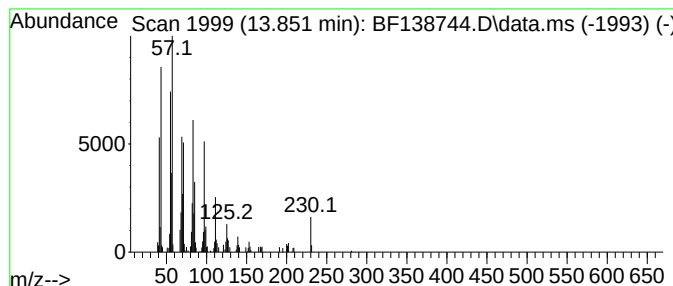
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	8.61 ng	192005	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2			Butyl docosyl ether	382	C26H54O	1000406-40-8	91
3			Propyl triacontyl ether	481	C33H68O	1000406-28-6	87
4			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	87
5			Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
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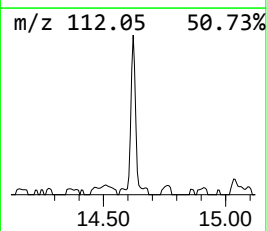
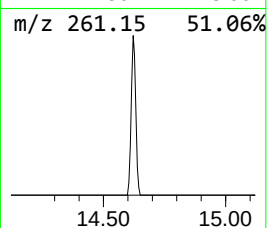
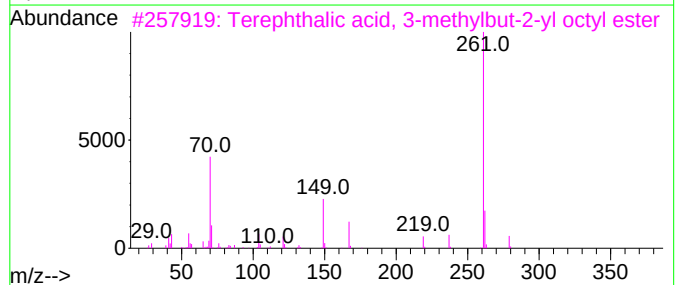
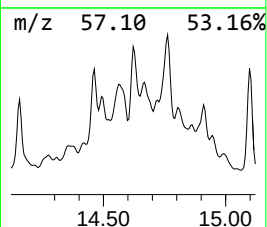
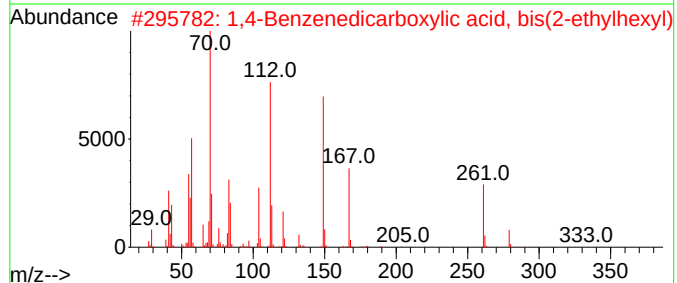
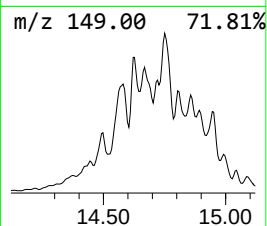
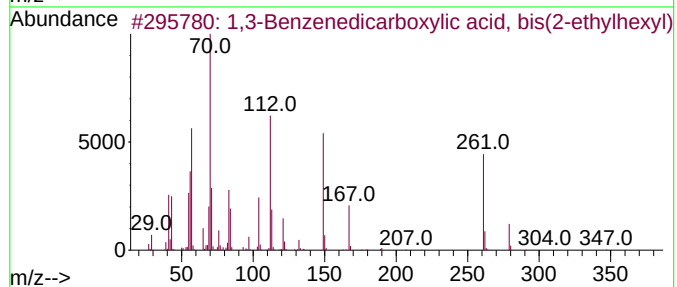
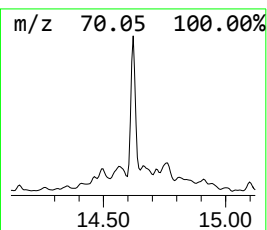
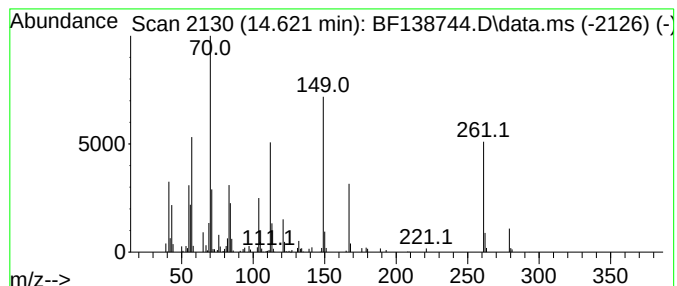
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,3-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	5.29 ng	117979	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	83
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	76
3			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	53
4			2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	38
5			Terephthalic acid, hept-3-yl oct...	376	C23H36O4	1000356-64-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
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Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

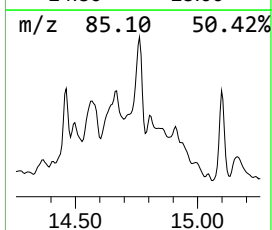
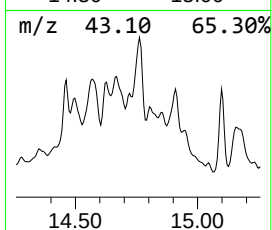
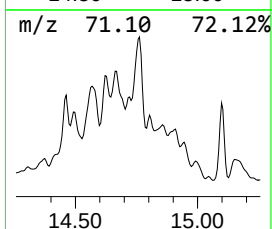
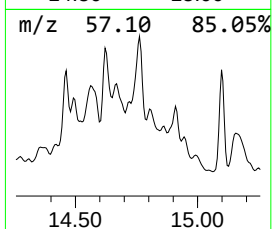
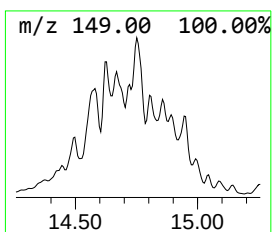
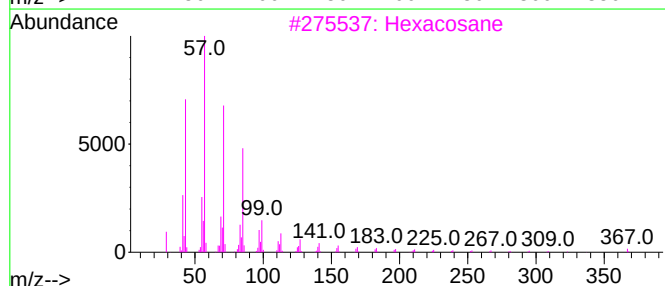
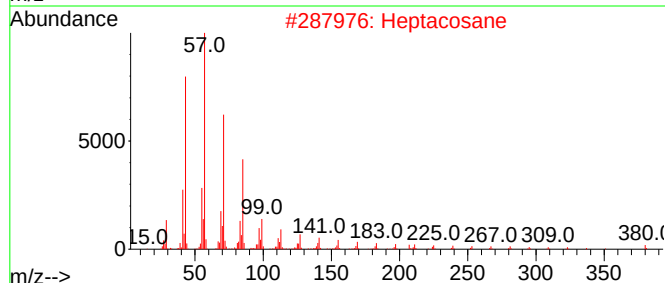
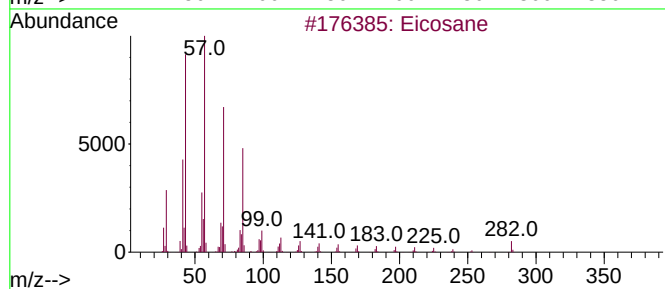
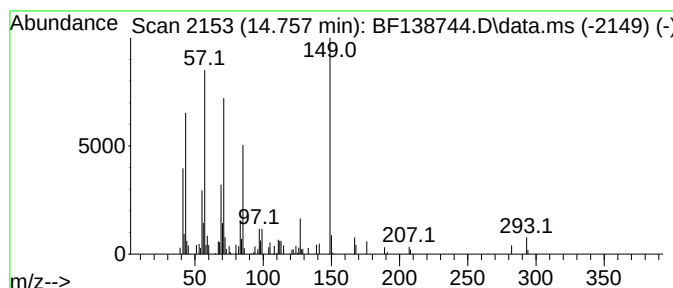
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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.757	4.88 ng	107075	Perylene-d12	15.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptacosane	380	C27H56	000593-49-7	46
3	Hexacosane	366	C26H54	000630-01-3	46
4	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	46
5	Nonadecane	268	C19H40	000629-92-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
355

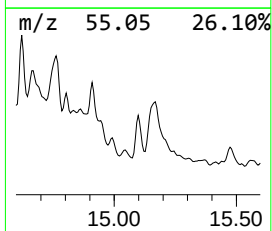
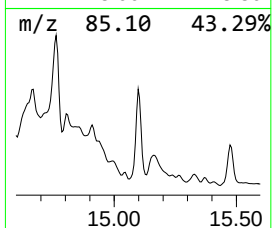
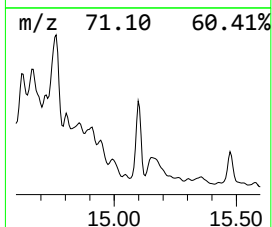
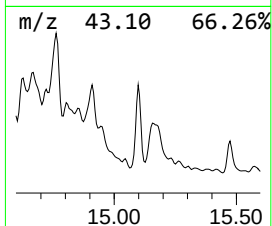
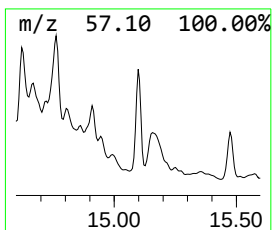
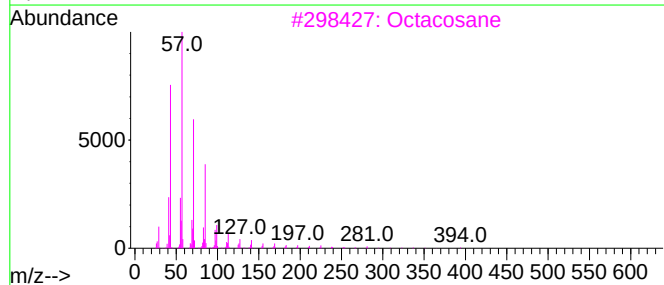
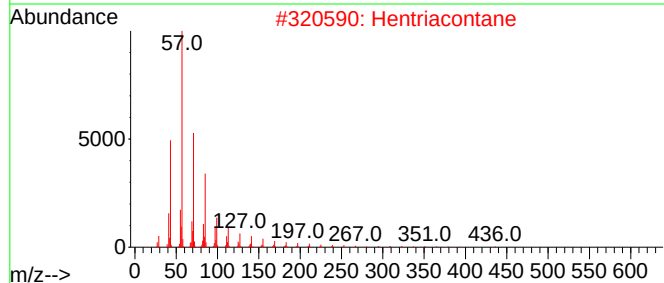
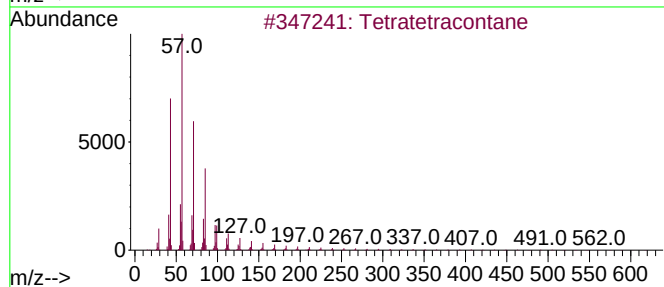
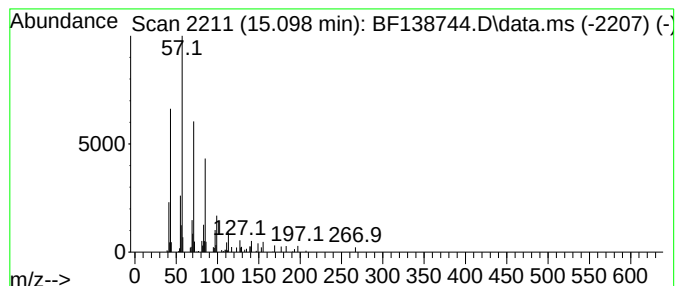
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetratetracontane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	2.45 ng	53832	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

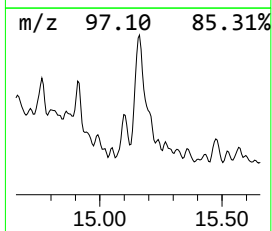
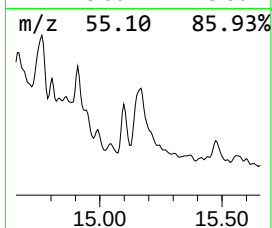
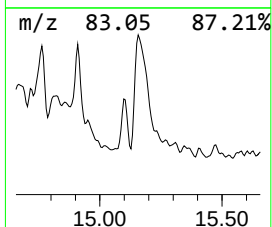
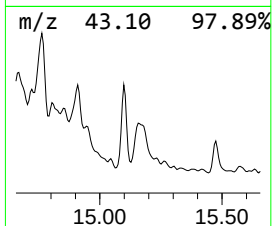
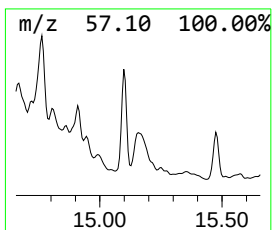
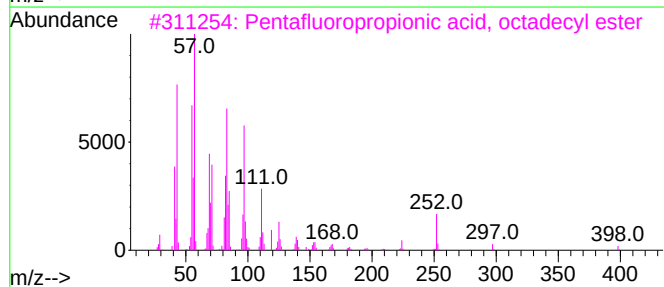
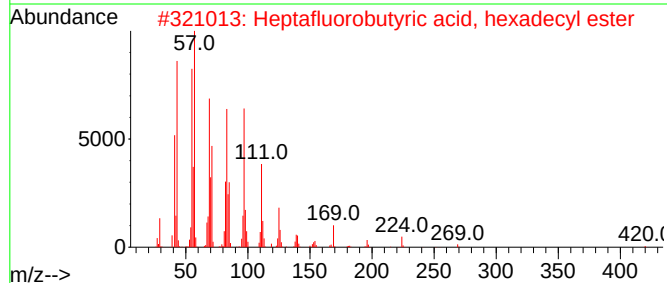
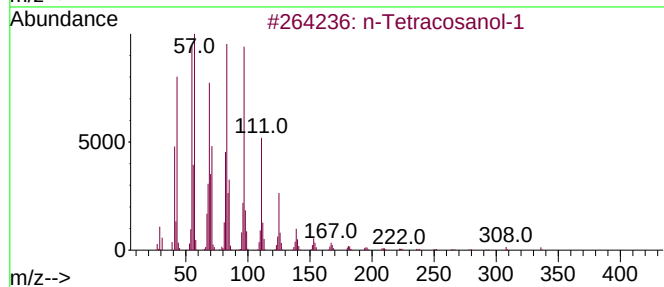
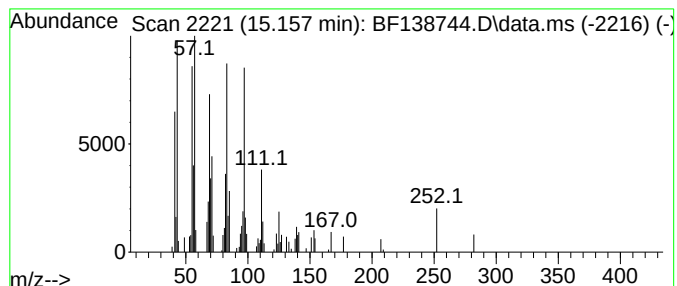
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.156	4.31 ng	94542	Perylene-d12	15.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	90
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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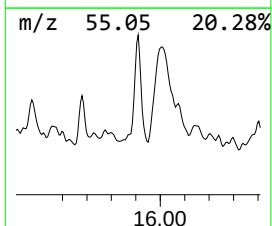
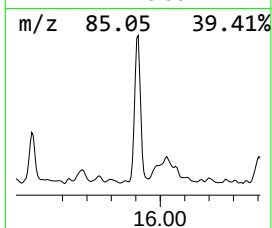
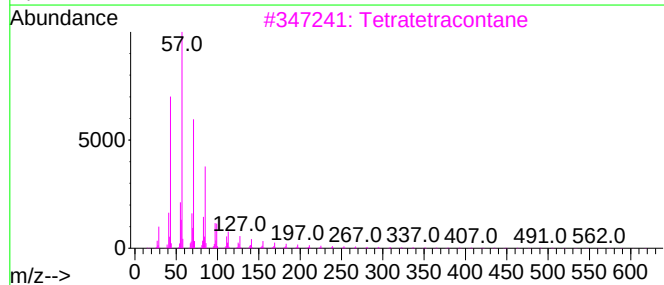
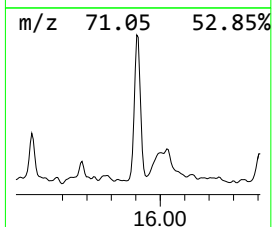
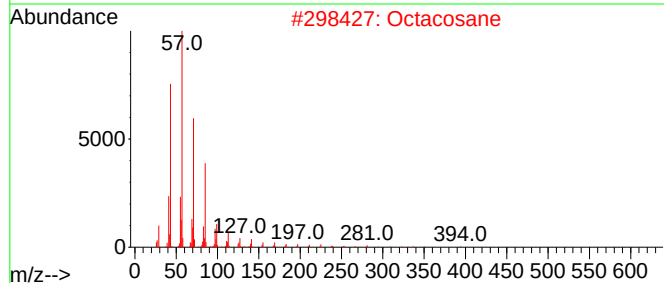
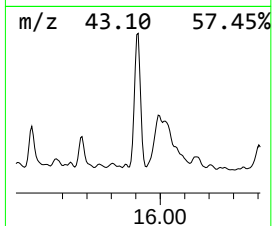
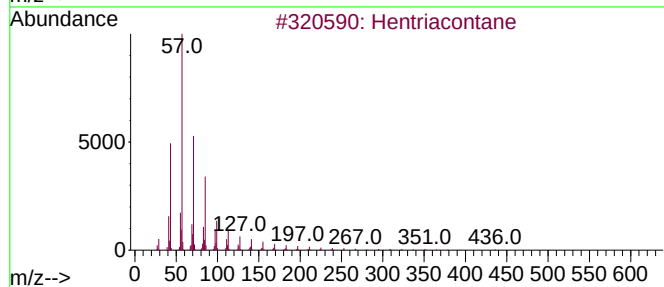
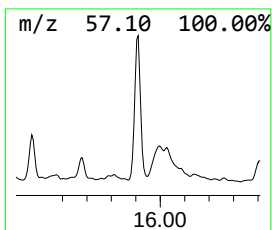
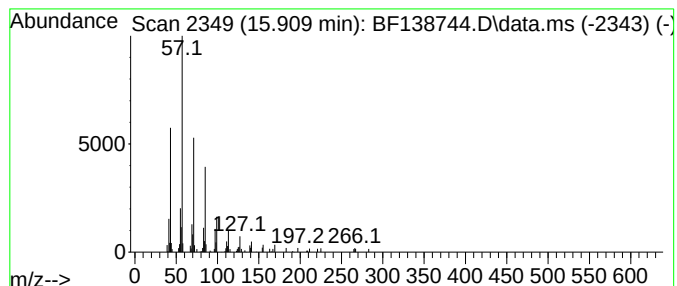
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.909	3.98 ng	87401	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			triacontane	422	C30H62	000638-68-6	91
5			Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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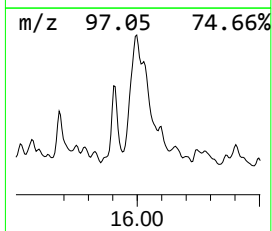
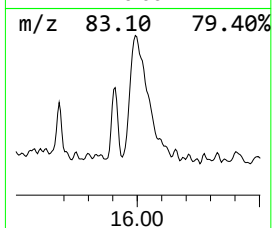
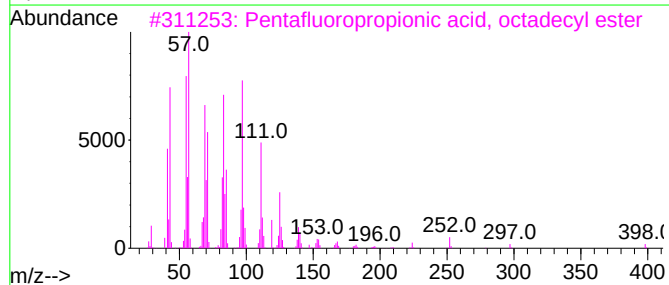
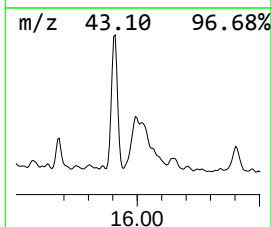
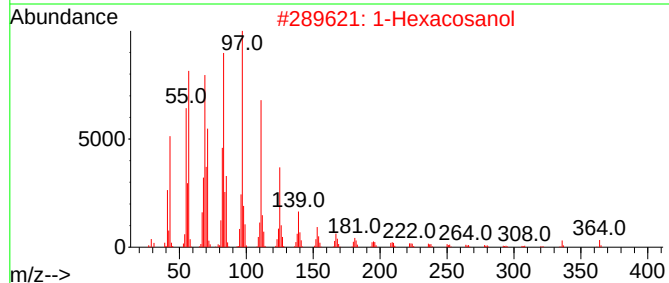
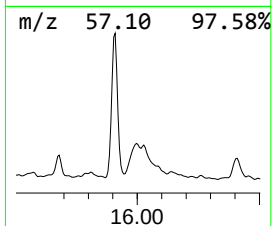
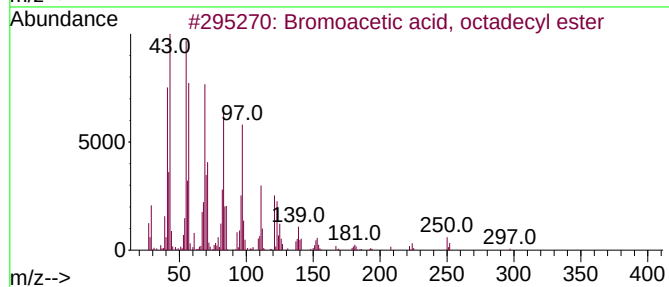
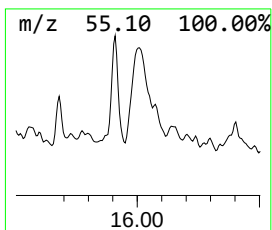
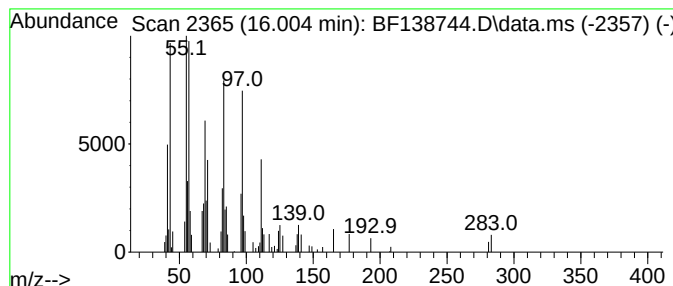
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Bromoacetic acid, octadecyl... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.003	2.62 ng	57427	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2		1-Hexacosanol	382	C26H54O	000506-52-5	87
3		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	80
4		Tetratriacontyl pentafluoropropionate	641	C37H69F5O2	1000351-81-5	68
5		Triacetyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
355

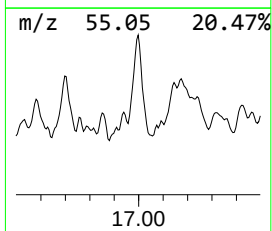
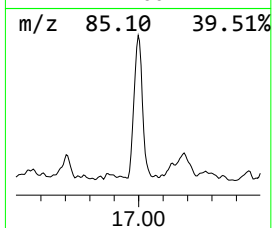
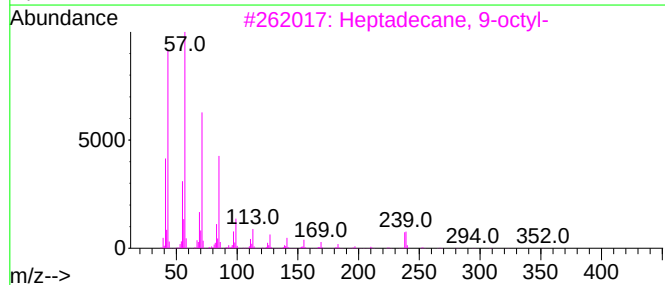
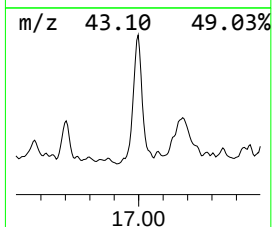
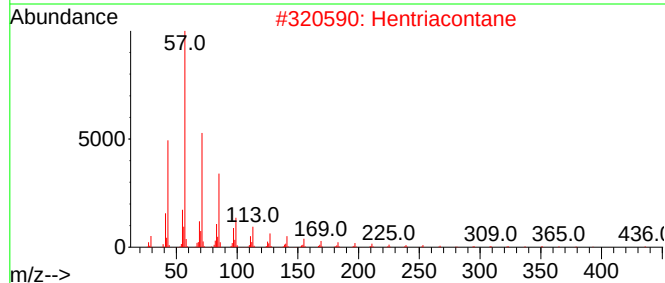
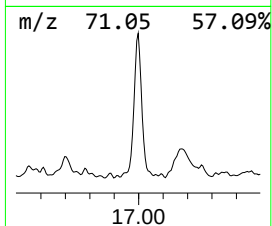
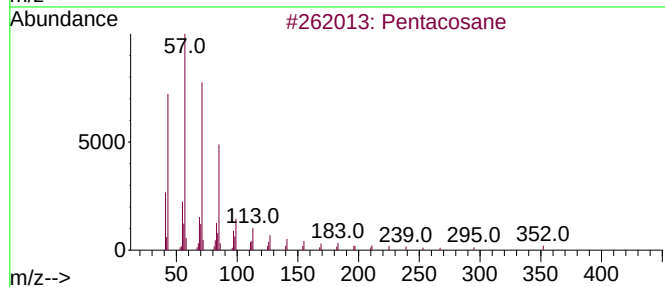
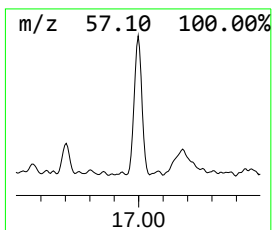
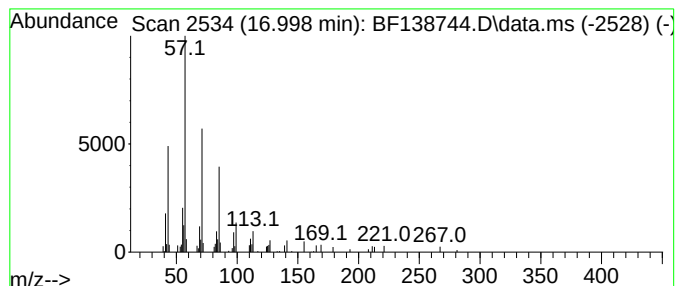
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.998	3.46 ng	75892	Perylene-d12	15.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosane	352	C25H52	000629-99-2	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Eicosane	282	C20H42	000112-95-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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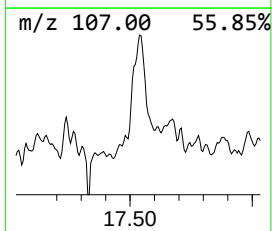
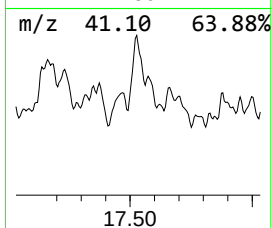
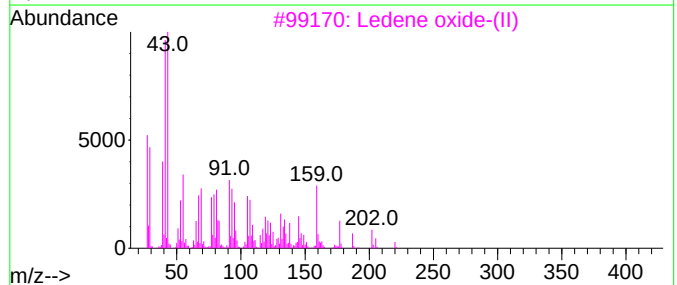
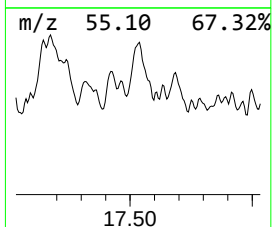
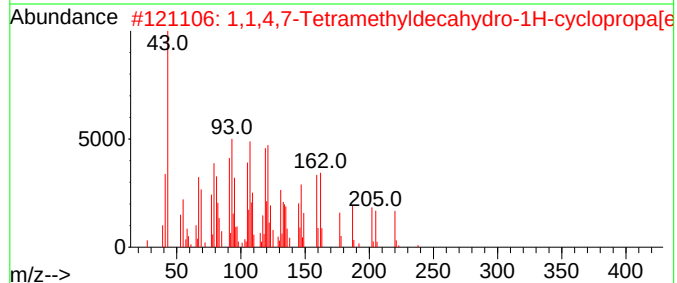
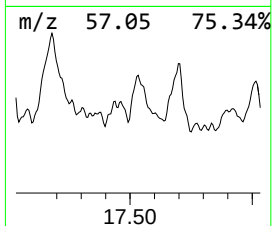
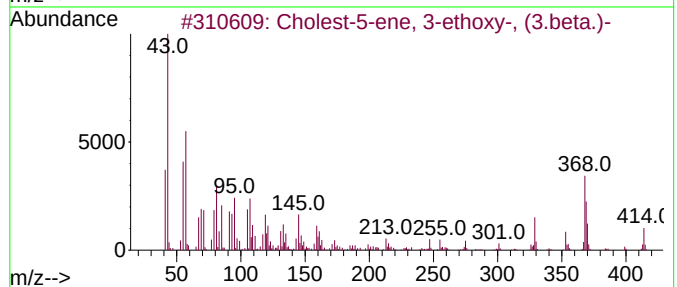
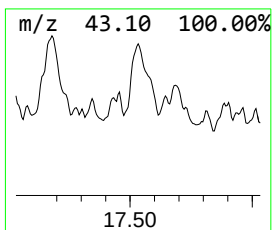
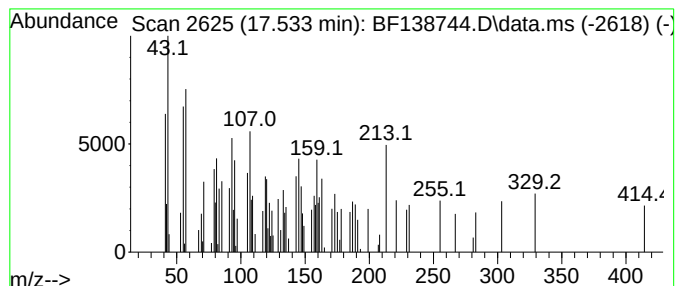
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Cholest-5-ene, 3-ethoxy-, (... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.533	2.83 ng	62116	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	60
2			1,1,4,7-Tetramethyldecahydro-1H-...	238	C15H26O2	1212211-43-2	30
3			Ledene oxide-(II)	220	C15H24O	1000159-36-7	10
4			Androst-5-en-7-one, 3-(acetyloxy...	358	C23H34O3	054549-89-2	10
5			Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
355

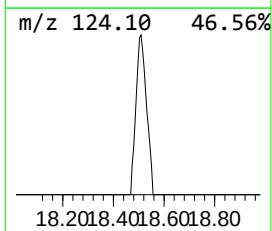
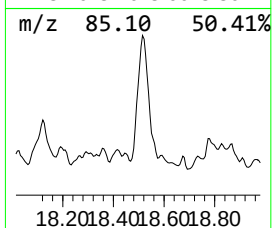
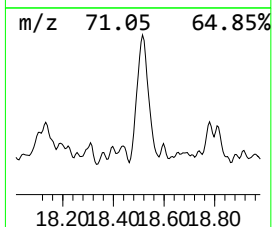
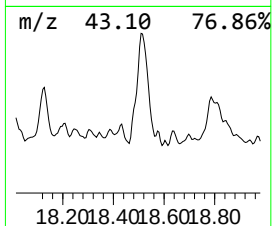
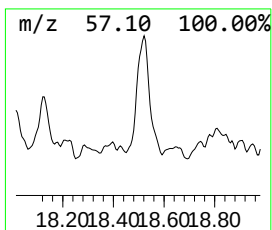
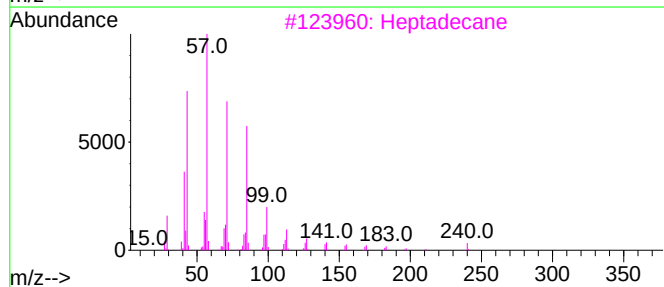
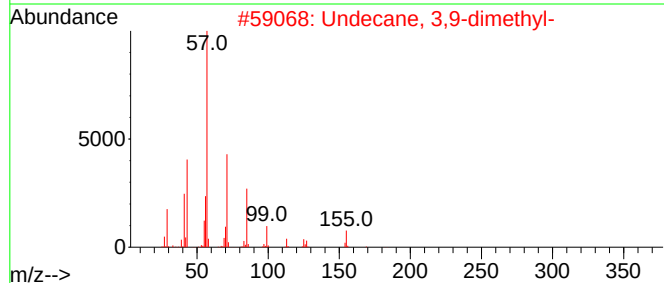
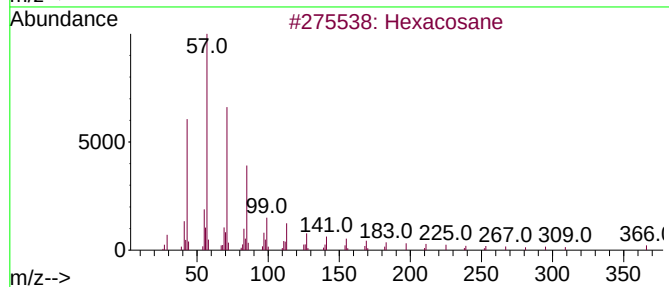
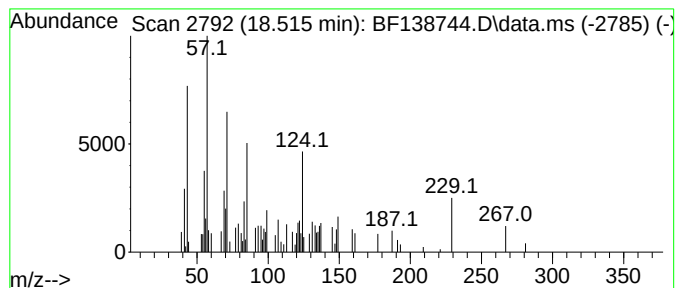
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown18.515 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.515	2.55 ng	56006	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	38
2			Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	35
3			Heptadecane	240	C17H36	000629-78-7	35
4			Hexadecane	226	C16H34	000544-76-3	35
5			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080224\
Data File : BF138744.D
Acq On : 02 Aug 2024 13:30
Operator : RC/JU
Sample : P3402-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
355

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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
Butane, 2-metho...	2.122	57.4	ng	1289630	1	6.845	449685	20.0
(S)-(+)-1,2-Pro...	3.363	2.9	ng	65841	1	6.845	449685	20.0
2-Pentanone, 4-...	5.063	5.1	ng	115616	1	6.845	449685	20.0
1-Phenoxypropan...	8.433	3.0	ng	93011	2	8.122	610927	20.0
unknown9.975	9.975	30.8	ng	1014410	3	9.875	659800	20.0
n-Hexadecanoic ...	11.892	3.3	ng	104693	4	11.363	641916	20.0
Benzene, 1,1'-(...	12.810	2.5	ng	56329	5	14.004	445871	20.0
2-Phenanthrenol...	13.374	3.7	ng	82928	5	14.004	445871	20.0
unknown13.410	13.410	3.8	ng	83725	5	14.004	445871	20.0
Pentadecafluoro...	13.851	8.6	ng	192005	5	14.004	445871	20.0
1,3-Benzenedica...	14.621	5.3	ng	117979	5	14.004	445871	20.0
Eicosane	14.757	4.9	ng	107075	6	15.468	439131	20.0
Tetratetracontane	15.098	2.5	ng	53832	6	15.468	439131	20.0
n-Tetracosanol-1	15.156	4.3	ng	94542	6	15.468	439131	20.0
Hentriacontane	15.909	4.0	ng	87401	6	15.468	439131	20.0
Bromoacetic aci...	16.003	2.6	ng	57427	6	15.468	439131	20.0
Pentacosane	16.998	3.5	ng	75892	6	15.468	439131	20.0
Cholest-5-ene, ...	17.533	2.8	ng	62116	6	15.468	439131	20.0
unknown18.515	18.515	2.5	ng	56006	6	15.468	439131	20.0