

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
 Data File : BF137761.D
 Acq On : 29 Apr 2024 21:41
 Operator : CG\JU
 Sample : P2294-05
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FOOT-PRINT-B-2

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-BF042324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137761.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	16	21	26	rVB3	57353	121465	2.08%	0.254%
2	2.428	52	58	64	rVB	397709	498202	8.53%	1.040%
3	3.704	271	275	282	rBV	30340	66186	1.13%	0.138%
4	5.687	607	612	615	rBV	5020178	4630614	79.26%	9.666%
5	6.675	774	780	783	rBV	4773978	4662185	79.80%	9.732%
6	7.063	842	846	849	rVB	1912167	1479497	25.33%	3.088%
7	7.622	936	941	944	rBV	3518291	3036819	51.98%	6.339%
8	8.233	1041	1045	1052	rBV	857069	696609	11.92%	1.454%
9	8.345	1060	1064	1067	rBV	2511905	1954842	33.46%	4.080%
10	8.645	1112	1115	1123	rVB	142674	127531	2.18%	0.266%
11	9.422	1242	1247	1250	rBV	6794673	5842035	100.00%	12.194%
12	10.104	1360	1363	1367	rBV	2235093	1970798	33.73%	4.114%
13	10.192	1373	1378	1385	rBV	2757104	3547121	60.72%	7.404%
14	10.657	1454	1457	1460	rBV	91285	72137	1.23%	0.151%
15	10.898	1494	1498	1501	rBV	3269840	2839017	48.60%	5.926%
16	11.004	1512	1516	1525	rVB5	44682	88753	1.52%	0.185%
17	11.604	1614	1618	1620	rBV	1852487	1653273	28.30%	3.451%
18	11.627	1620	1622	1625	rVV	515053	420973	7.21%	0.879%
19	11.674	1625	1630	1633	rVV	147374	129167	2.21%	0.270%
20	12.104	1700	1703	1706	rBV	463889	413982	7.09%	0.864%
21	12.133	1706	1708	1712	rVB2	121418	105804	1.81%	0.221%
22	12.216	1719	1722	1725	rBV2	146030	170667	2.92%	0.356%
23	12.657	1791	1797	1801	rBV2	85480	176984	3.03%	0.369%
24	12.827	1822	1826	1829	rBV	1000174	854554	14.63%	1.784%
25	12.857	1829	1831	1833	rVV2	100989	73195	1.25%	0.153%
26	12.892	1833	1837	1843	rVV4	78206	101352	1.73%	0.212%
27	13.051	1861	1864	1870	rVB	835045	783596	13.41%	1.636%
28	13.186	1884	1887	1891	rVB	4587680	4156456	71.15%	8.676%
29	13.262	1897	1900	1904	rBV3	61706	100435	1.72%	0.210%
30	13.380	1917	1920	1922	rVB	114999	99421	1.70%	0.208%
31	13.445	1928	1931	1933	rVB	146080	110147	1.89%	0.230%
32	13.480	1935	1937	1940	rVB2	79045	74828	1.28%	0.156%
33	13.580	1951	1954	1956	rBV	64171	69489	1.19%	0.145%
34	14.033	2028	2031	2033	rBV2	79413	85503	1.46%	0.178%
35	14.074	2035	2038	2050	rVB3	351762	612930	10.49%	1.279%
36	14.215	2059	2062	2064	rBV2	76121	69983	1.20%	0.146%

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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-BF042324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.251	2064	2068	2071	rVV2	1648462	1804588	30.89%	3.767%
38	14.274	2071	2072	2079	rVB	388083	353427	6.05%	0.738%
39	14.392	2090	2092	2095	rBV	95177	72413	1.24%	0.151%
40	14.704	2142	2145	2147	rBV	288740	275299	4.71%	0.575%
41	15.204	2227	2230	2234	rVB	193132	213890	3.66%	0.446%
42	15.351	2251	2255	2259	rBV	284681	485058	8.30%	1.012%
43	15.409	2262	2265	2270	rVB	676816	797395	13.65%	1.664%
44	15.686	2310	2312	2320	rVB	159669	195582	3.35%	0.408%
45	15.756	2321	2324	2330	rVB	240980	309811	5.30%	0.647%
46	15.827	2332	2336	2340	rBV	792587	1009613	17.28%	2.107%
47	16.327	2417	2421	2426	rVB	326044	493755	8.45%	1.031%

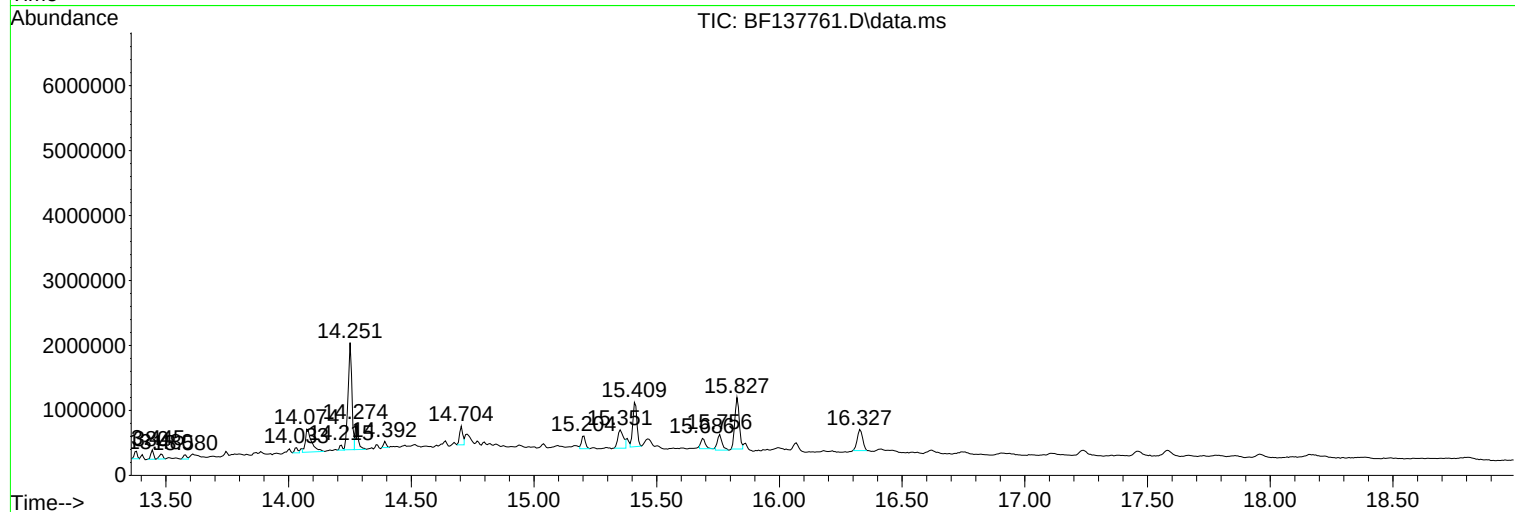
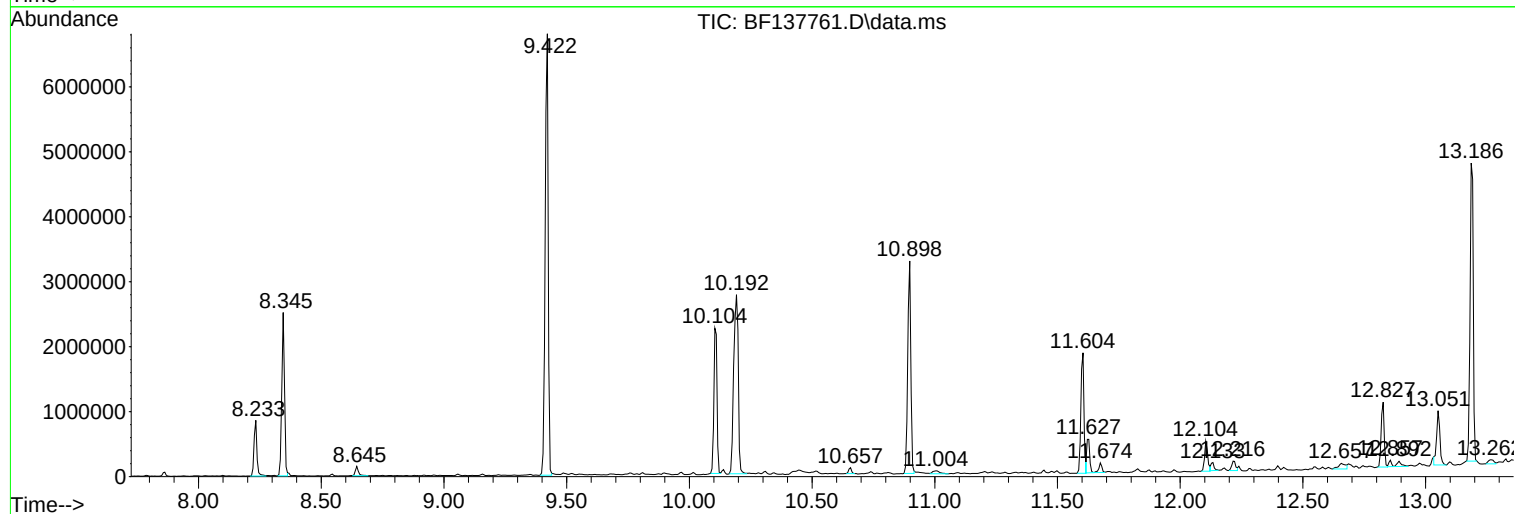
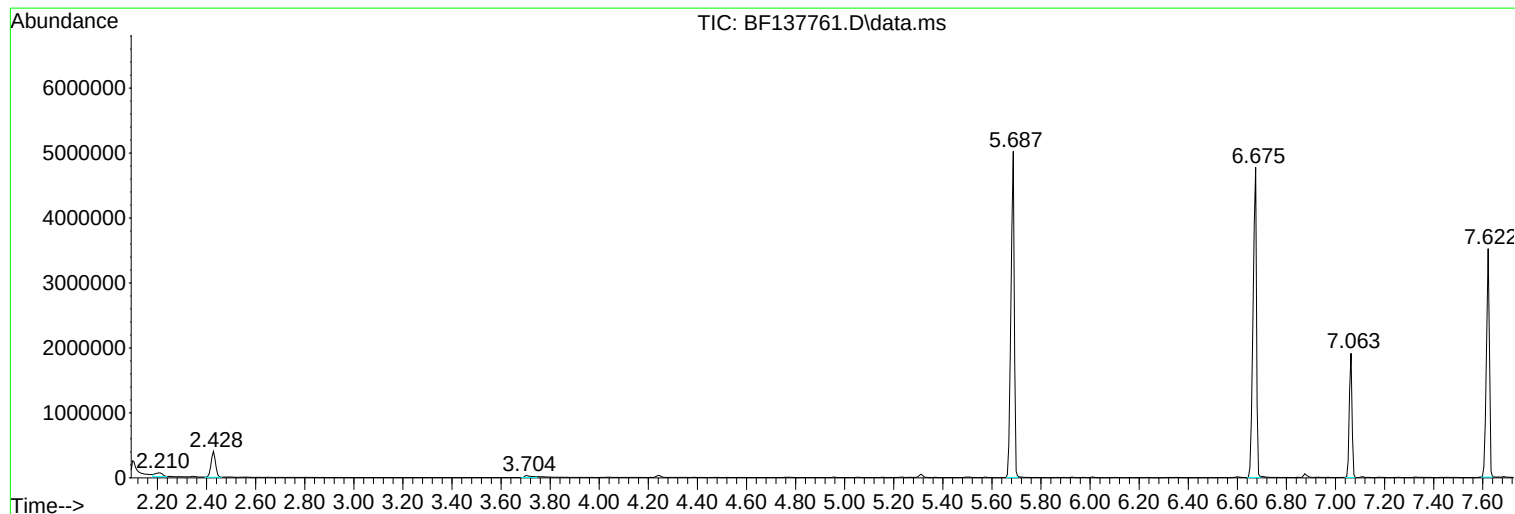
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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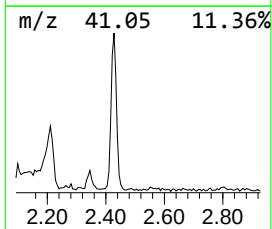
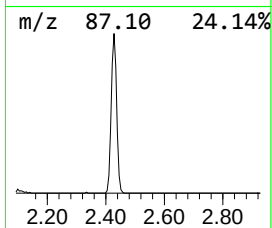
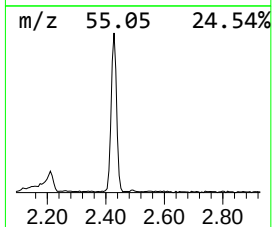
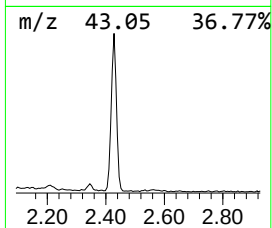
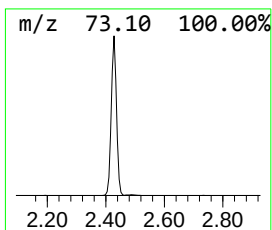
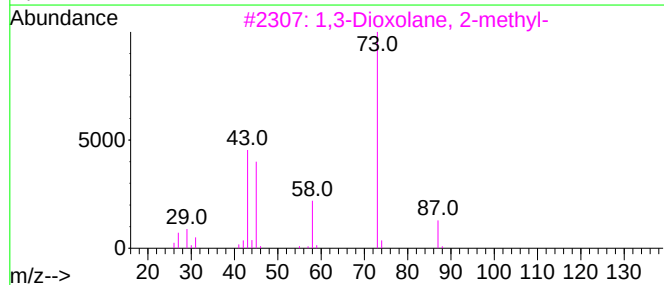
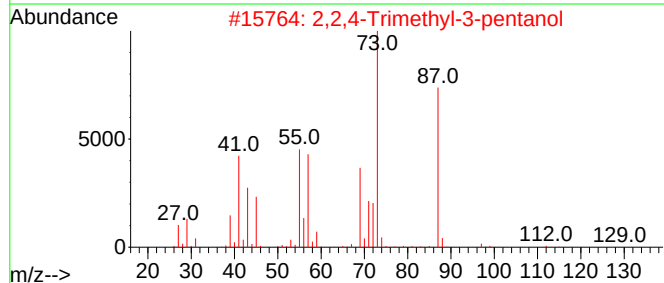
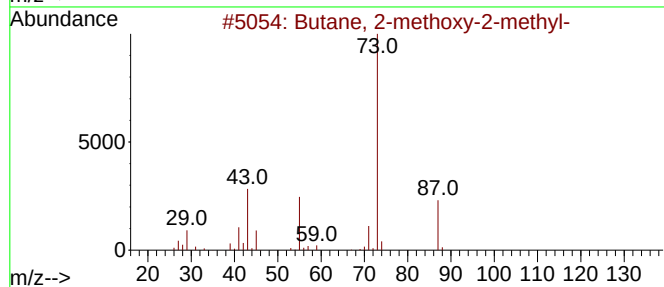
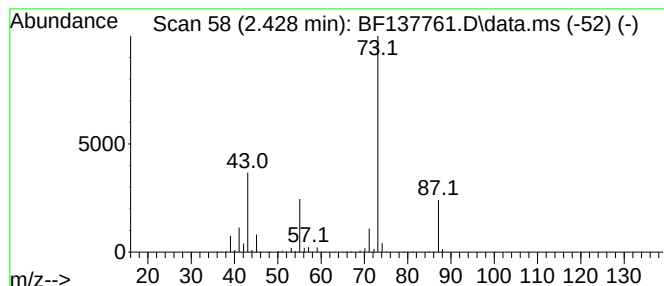
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.428	6.73 ng	498202	1,4-Dichlorobenzene-d4	7.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
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	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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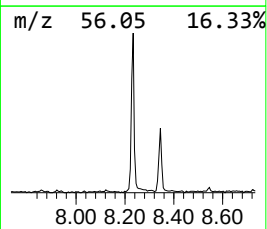
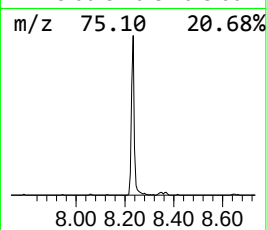
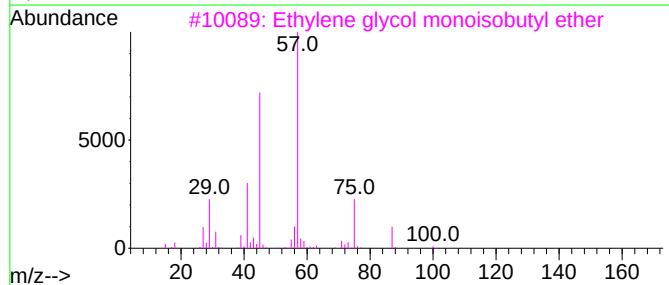
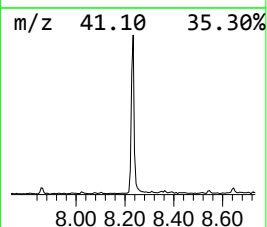
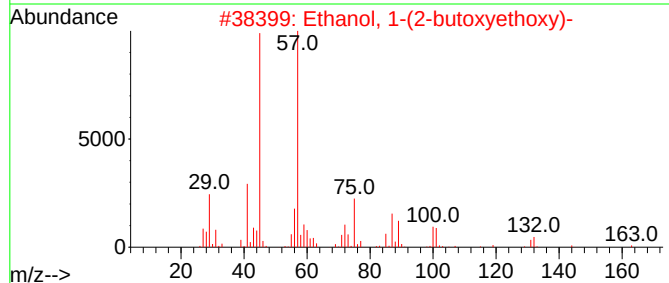
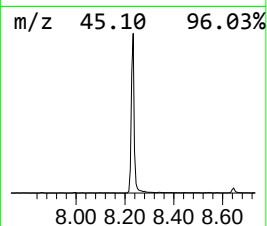
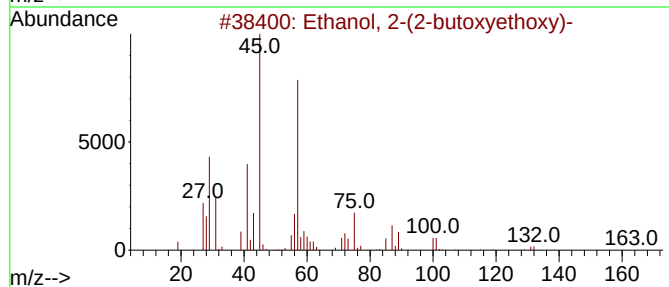
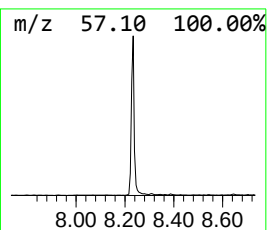
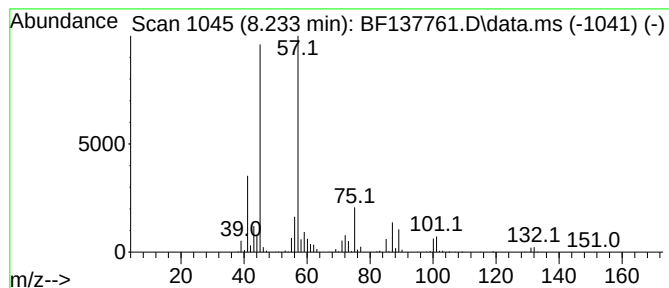
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.233	7.13 ng	696609	Naphthalene-d8	8.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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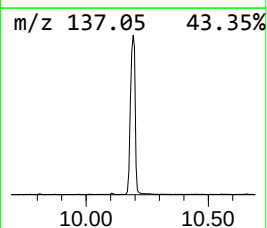
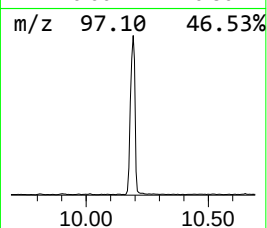
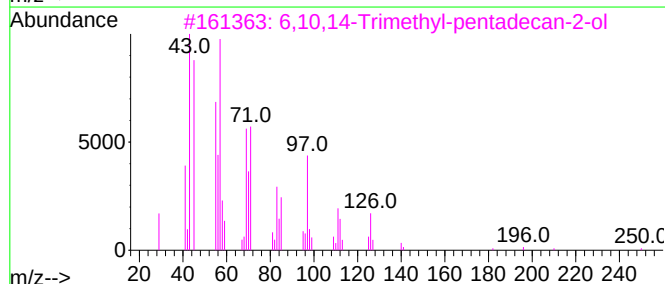
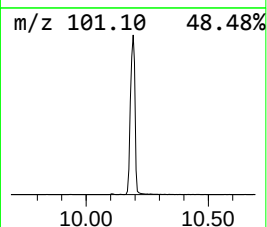
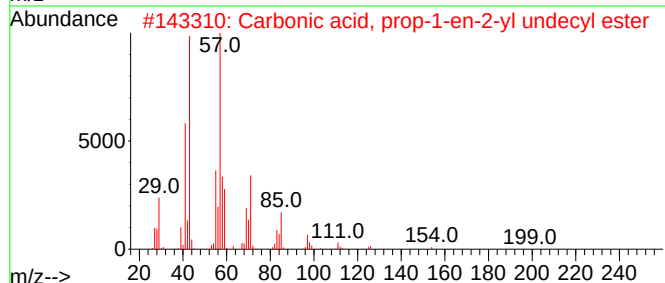
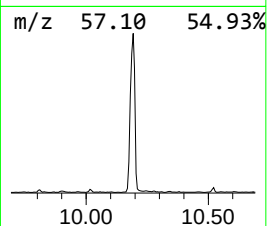
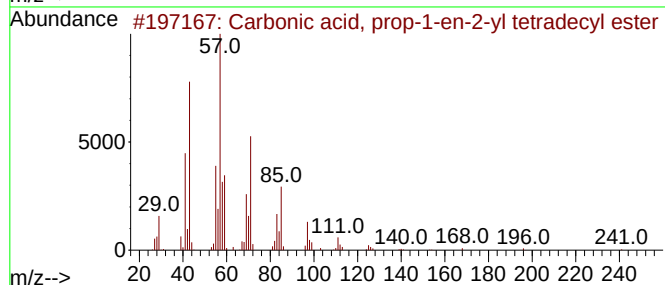
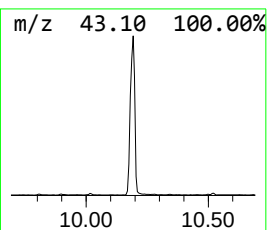
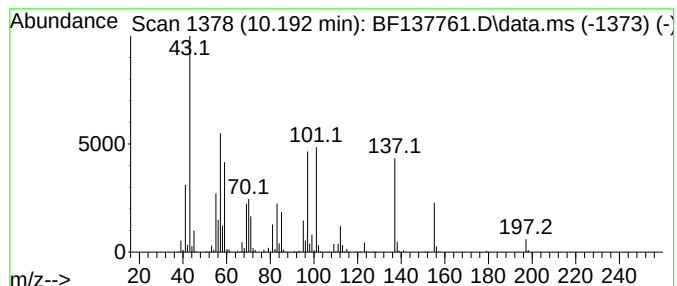
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown10.192 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.192	36.00 ng	3547120	Acenaphthene-d10	10.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	12
2			Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	10
3			6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	10
4			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	10
5			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	10



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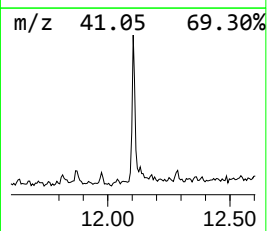
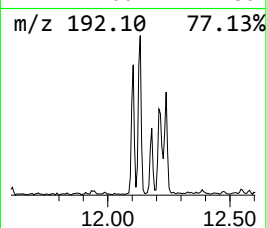
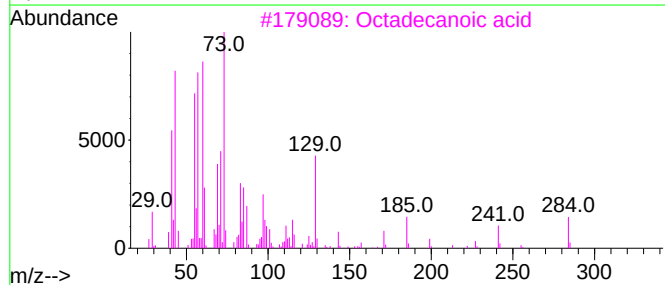
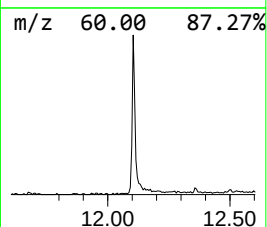
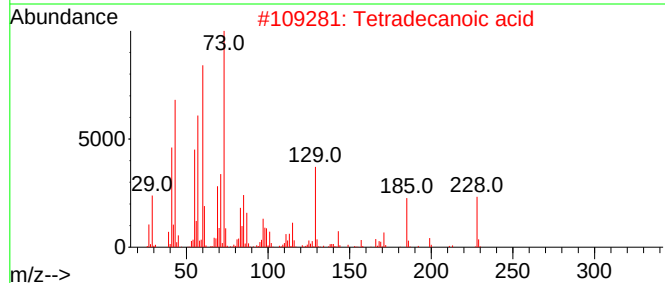
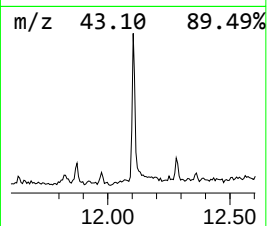
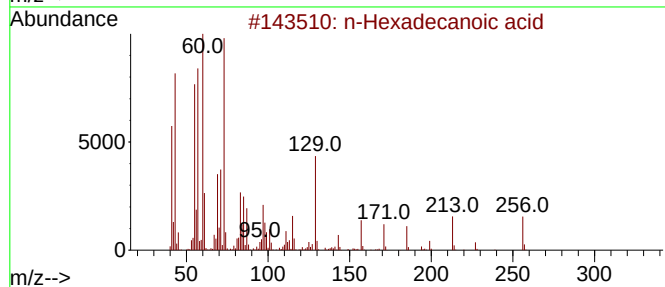
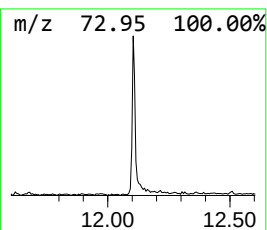
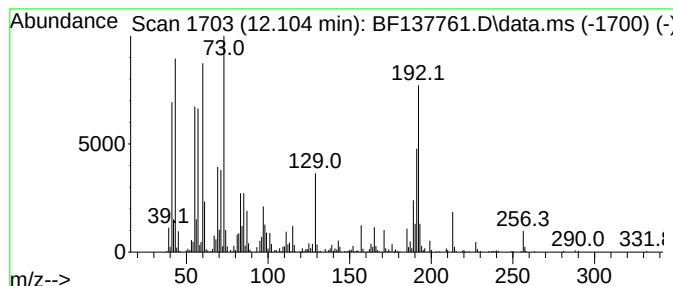
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	5.01 ng	413982	Phenanthrene-d10	11.604

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		Octadecanoic acid	284	C18H36O2	000057-11-4	87
4		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	74
5		1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	74



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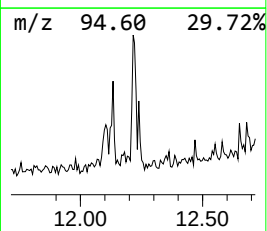
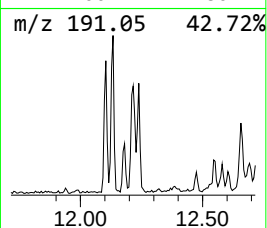
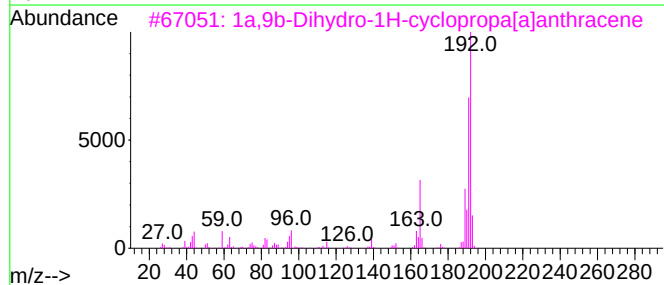
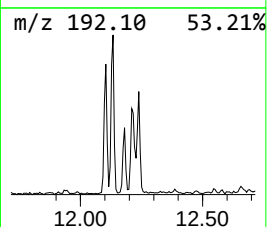
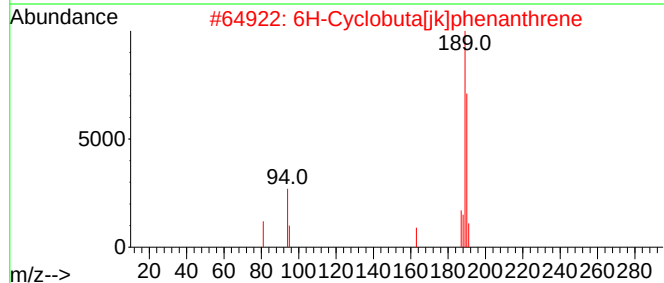
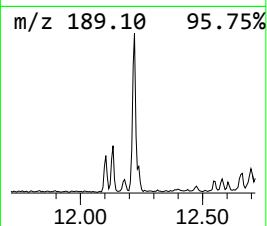
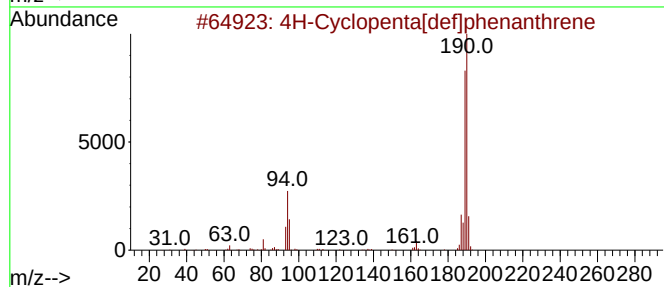
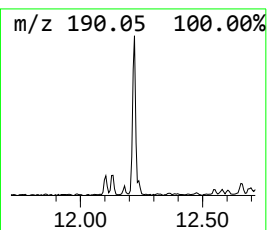
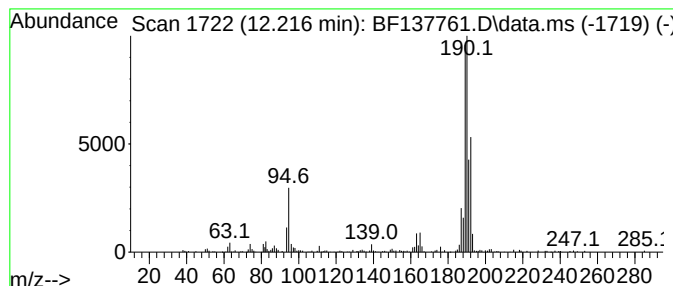
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.216	2.06 ng	170667	Phenanthrene-d10	11.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	92
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
3			1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	18
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	14
5			Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137761.D
Acq On : 29 Apr 2024 21:41
Operator : CG\JU
Sample : P2294-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FOOT-PRINT-B-2

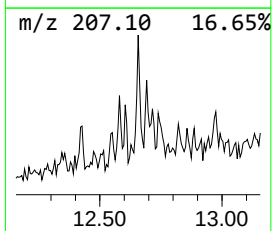
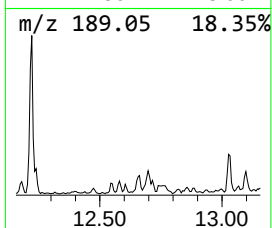
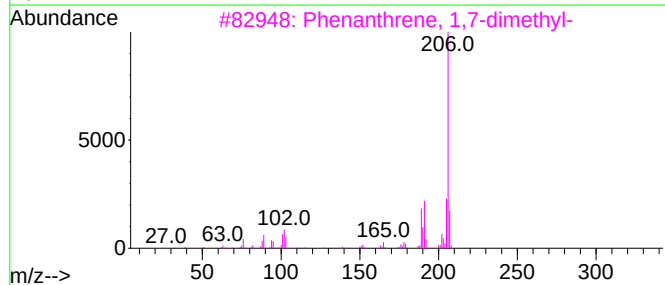
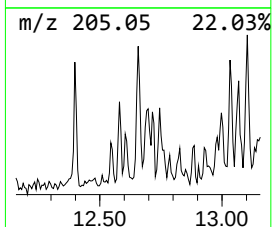
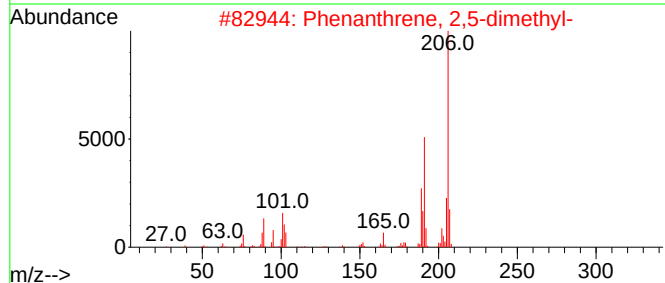
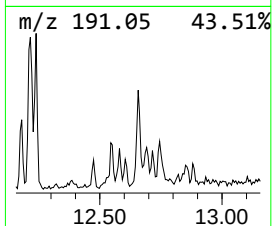
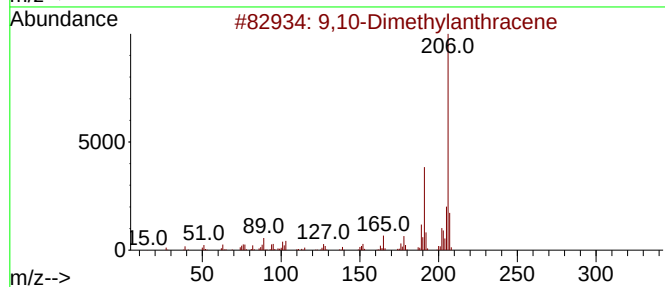
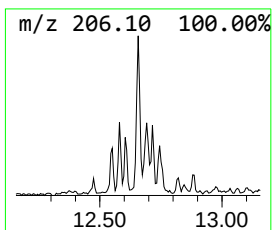
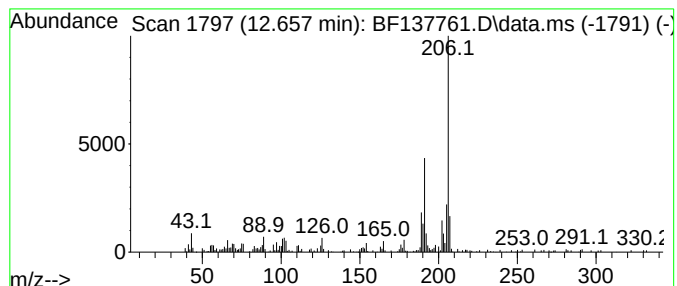
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,10-Dimethylantracene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	2.14 ng	176984	Phenanthrene-d10	11.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,10-Dimethylantracene	206	C16H14	000781-43-1	97
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	96
3			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	94
4			di-p-Tolylacetylene	206	C16H14	002789-88-0	90
5			Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137761.D
Acq On : 29 Apr 2024 21:41
Operator : CG\JU
Sample : P2294-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FOOT-PRINT-B-2

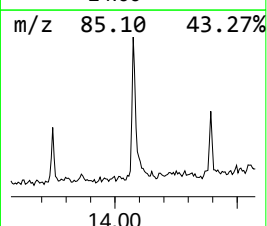
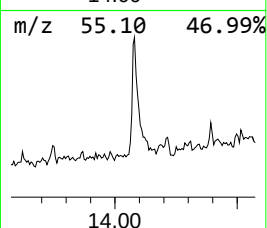
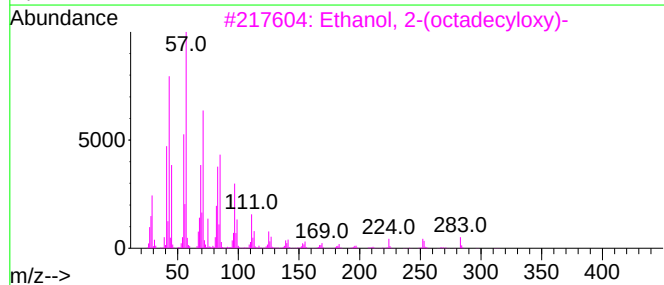
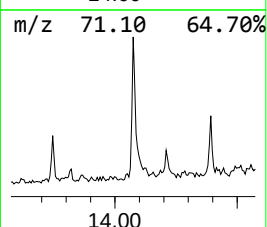
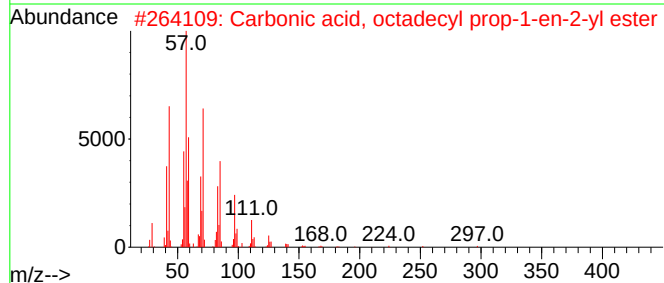
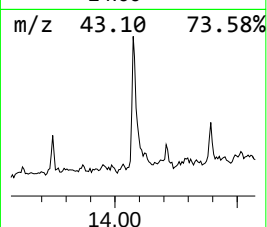
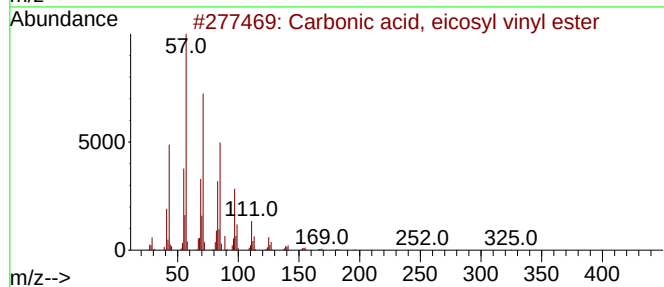
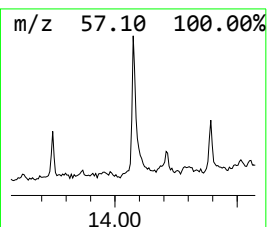
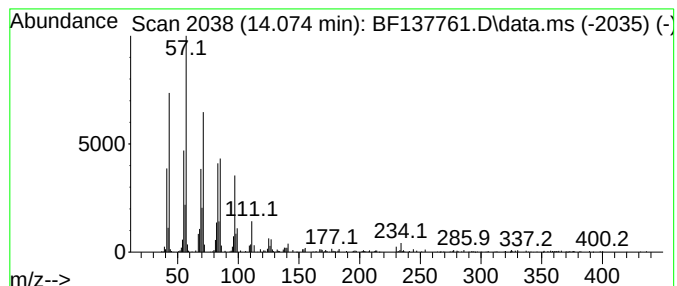
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Carbonic acid, eicosyl vinyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	6.79 ng	612930	Chrysene-d12	14.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3			Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	90
4			Carbonic acid, decyl pentadecyl ...	412	C26H52O3	1000383-16-4	87
5			Carbonic acid, decyl tetradecyl ...	398	C25H50O3	1010383-16-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137761.D
Acq On : 29 Apr 2024 21:41
Operator : CG\JU
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ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
FOOT-PRINT-B-2

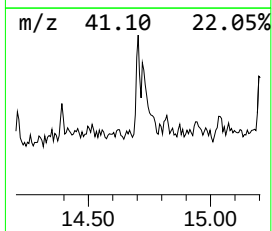
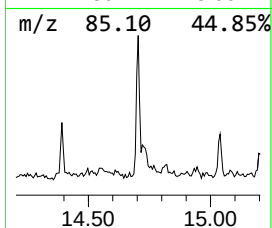
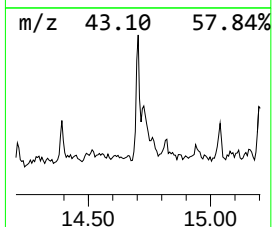
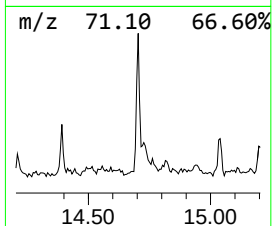
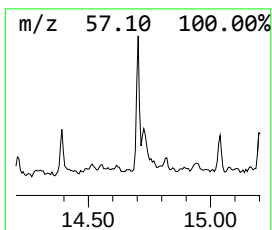
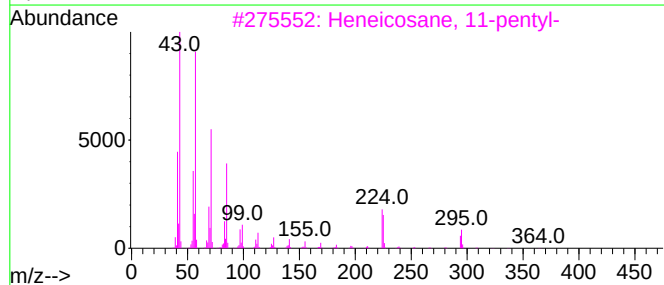
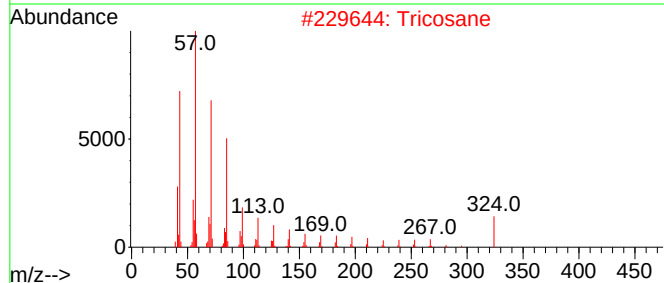
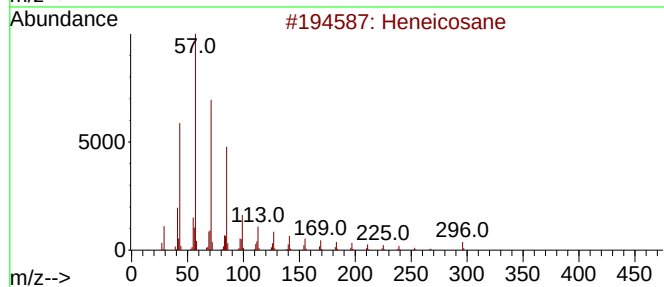
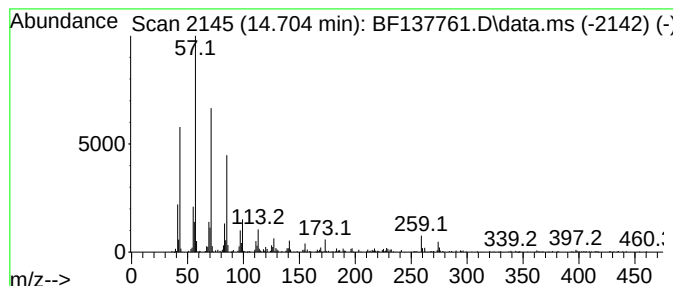
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.704	3.05 ng	275299	Chrysene-d12	14.251

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	96
2		Tricosane	324	C23H48	000638-67-5	95
3		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
4		Hexacosane	366	C26H54	000630-01-3	93
5		Docosane, 9-butyl-	366	C26H54	055282-14-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137761.D
Acq On : 29 Apr 2024 21:41
Operator : CG\JU
Sample : P2294-05
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ALS Vial : 17 Sample Multiplier: 1

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FOOT-PRINT-B-2

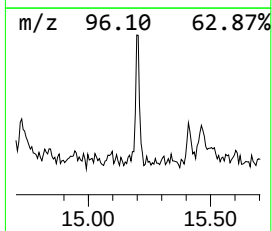
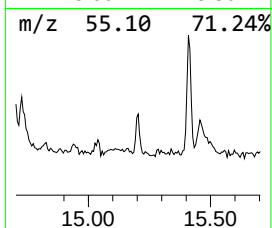
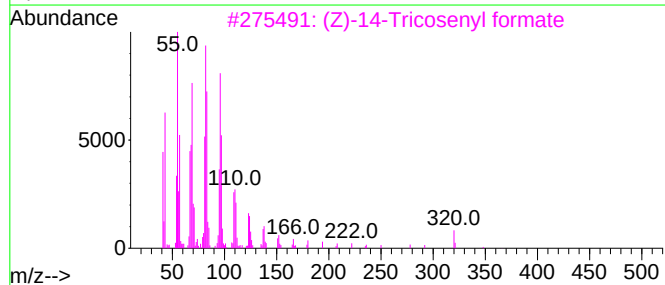
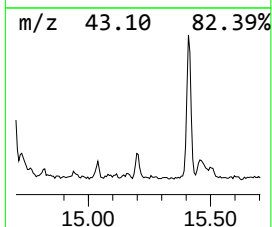
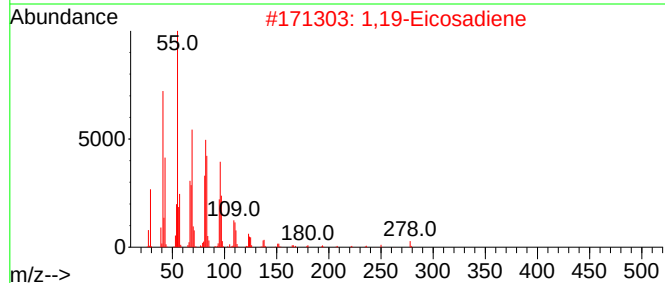
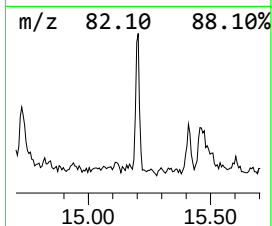
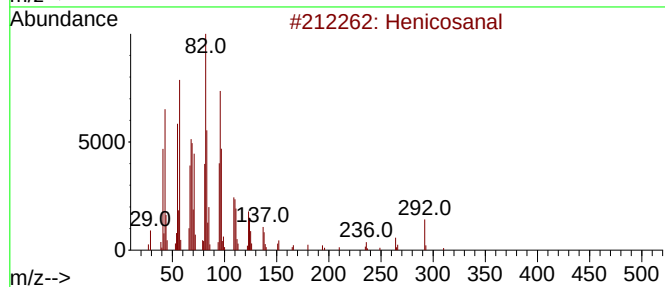
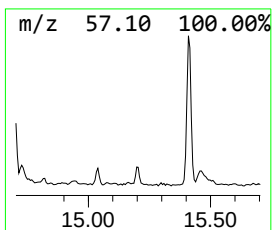
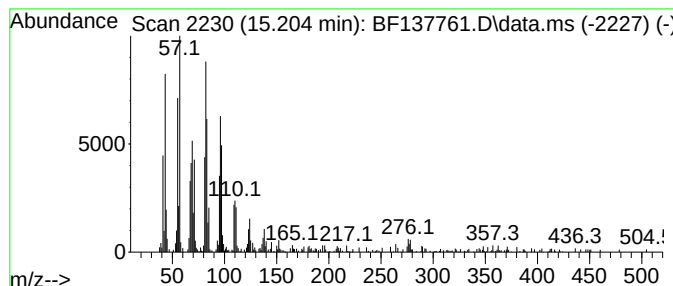
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Henicosanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	4.24 ng	213890	Perylene-d12	15.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Henicosanal	310	C21H42O	051227-32-8	93
2			1,19-Eicosadiene	278	C20H38	014811-95-1	93
3			(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	93
4			Octadecanal	268	C18H36O	000638-66-4	91
5			Pentacosanal	366	C25H50O	058196-28-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137761.D
Acq On : 29 Apr 2024 21:41
Operator : CG\JU
Sample : P2294-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FOOT-PRINT-B-2

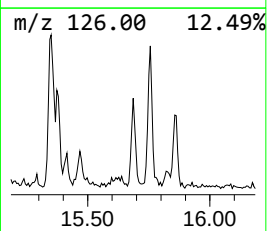
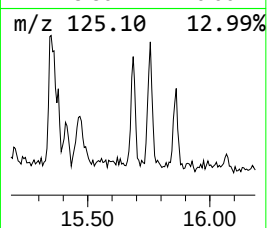
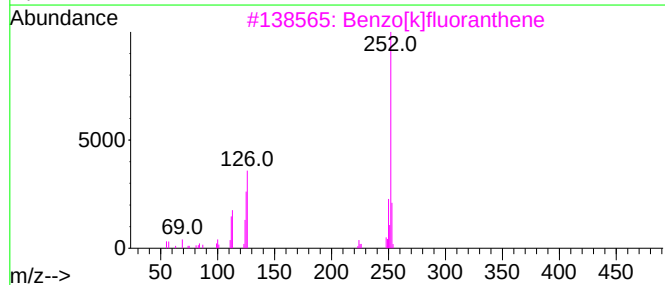
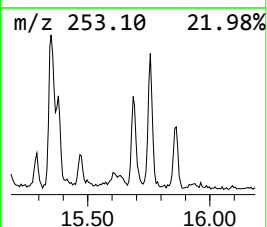
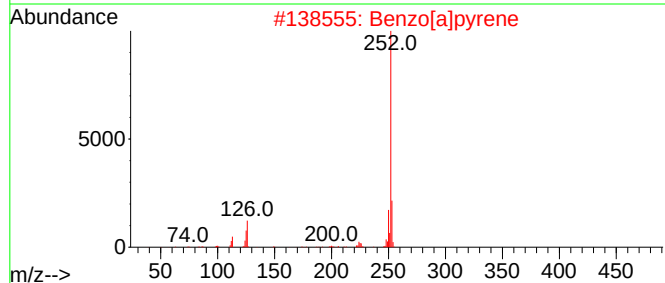
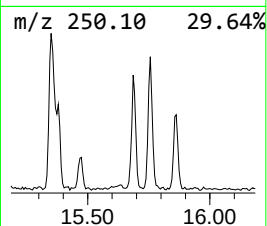
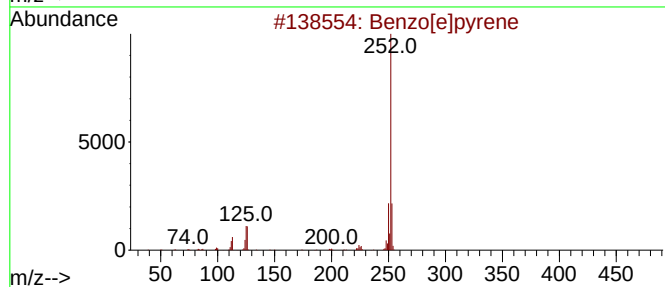
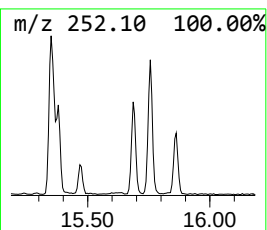
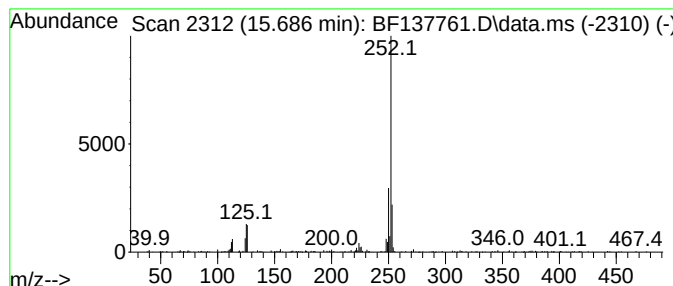
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.686	3.87 ng	195582	Perylene-d12	15.827

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	97
2		Benzo[a]pyrene	252	C20H12	000050-32-8	96
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4		Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
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Acq On : 29 Apr 2024 21:41
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Sample : P2294-05
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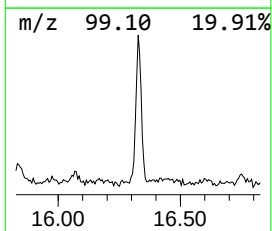
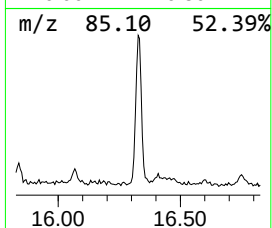
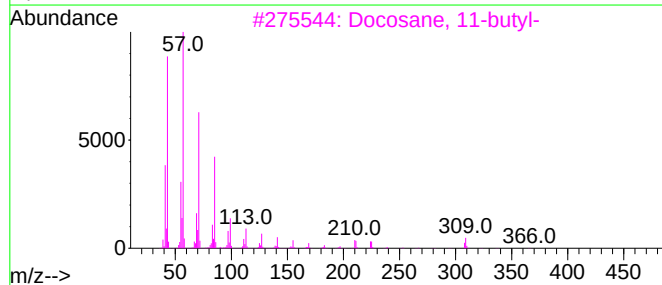
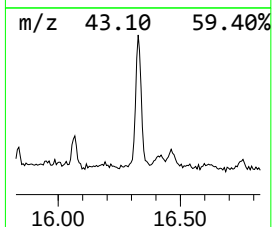
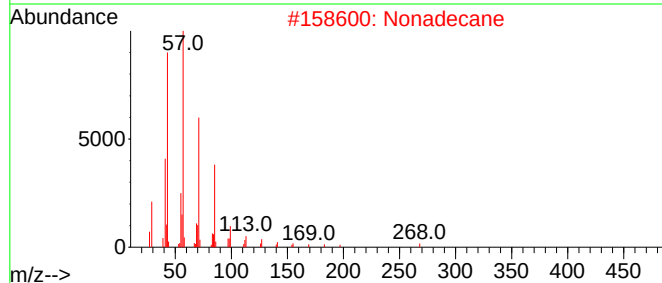
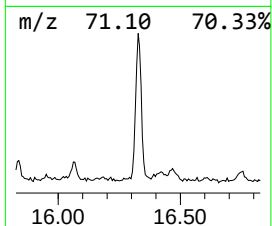
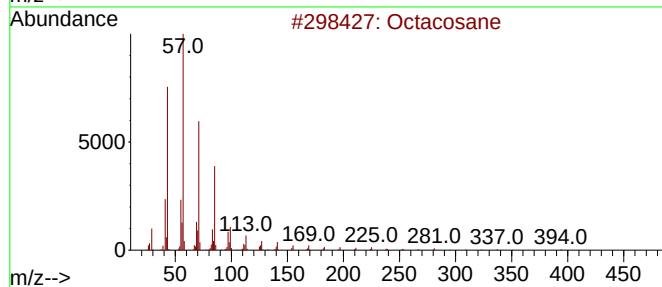
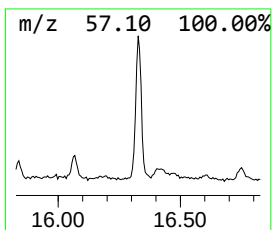
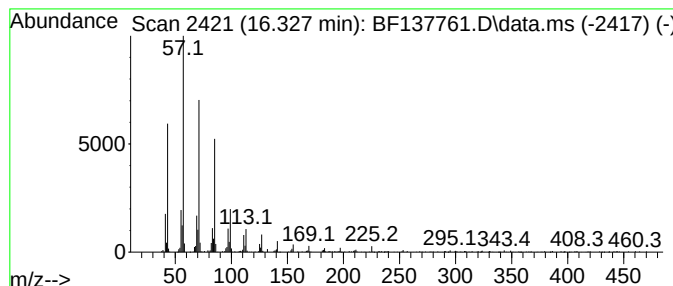
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.327	9.78 ng	493755	Perylene-d12	15.827	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	97
2	Nonadecane	268	C19H40	000629-92-5	94
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
5	3-Methylheptacosane	394	C28H58	014167-66-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137761.D
Acq On : 29 Apr 2024 21:41
Operator : CG\JU
Sample : P2294-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.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
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Ethanol, 2-(2-b...	8.233	7.1	ng	696609	2	8.345	1954840	20.0
unknown10.192	10.192	36.0	ng	3547120	3	10.110	1970800	20.0
n-Hexadecanoic ...	12.104	5.0	ng	413982	4	11.604	1653270	20.0
4H-Cyclopenta[d...	12.216	2.1	ng	170667	4	11.604	1653270	20.0
9,10-Dimethylan...	12.657	2.1	ng	176984	4	11.604	1653270	20.0
Carbonic acid, ...	14.074	6.8	ng	612930	5	14.251	1804590	20.0
Heneicosane	14.704	3.0	ng	275299	5	14.251	1804590	20.0
Henicosanal	15.204	4.2	ng	213890	6	15.827	1009610	20.0
Benzo[e]pyrene	15.686	3.9	ng	195582	6	15.827	1009610	20.0
Octacosane	16.327	9.8	ng	493755	6	15.827	1009610	20.0