

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
 Data File : BF137762.D
 Acq On : 29 Apr 2024 22:14
 Operator : CG\JU
 Sample : P2294-06
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FOOT-PRINT-B-3

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: BF137762.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.434	54	59	65	rVB	380743	512236	8.51%	1.126%
2	3.710	273	276	282	rBV	48369	92819	1.54%	0.204%
3	5.687	607	612	615	rBV	4823737	4840026	80.44%	10.643%
4	6.675	774	780	783	rBV	4804206	4819109	80.09%	10.597%
5	7.063	842	846	849	rBV	1965577	1508819	25.08%	3.318%
6	7.622	936	941	944	rBV	3555301	3144788	52.26%	6.915%
7	8.233	1041	1045	1056	rBV	900096	735152	12.22%	1.617%
8	8.345	1060	1064	1067	rBV	2506758	1993562	33.13%	4.384%
9	8.645	1112	1115	1123	rVB	148426	130961	2.18%	0.288%
10	9.422	1242	1247	1250	rBV	7191895	6017119	100.00%	13.231%
11	10.104	1360	1363	1367	rBV	2291407	2035242	33.82%	4.475%
12	10.139	1367	1369	1372	rVB	126360	92114	1.53%	0.203%
13	10.186	1372	1377	1384	rVB	199350	274993	4.57%	0.605%
14	10.310	1395	1398	1401	rVB	77532	68438	1.14%	0.150%
15	10.657	1453	1457	1463	rVB	143992	137805	2.29%	0.303%
16	10.898	1494	1498	1501	rBV	3431227	2929842	48.69%	6.442%
17	11.598	1614	1617	1620	rBV	1817421	1706934	28.37%	3.753%
18	11.621	1620	1621	1625	rVV	819857	635556	10.56%	1.398%
19	11.674	1625	1630	1633	rVV	269844	223713	3.72%	0.492%
20	11.827	1649	1656	1661	rBV	56377	84439	1.40%	0.186%
21	12.104	1699	1703	1706	rBV	593156	512348	8.51%	1.127%
22	12.127	1706	1707	1712	rVB2	140051	119021	1.98%	0.262%
23	12.216	1718	1722	1725	rBV2	171884	191676	3.19%	0.421%
24	12.651	1793	1796	1799	rBV	59651	71757	1.19%	0.158%
25	12.821	1821	1825	1829	rBV	1269273	1047671	17.41%	2.304%
26	12.892	1833	1837	1843	rVV3	115262	135072	2.24%	0.297%
27	13.051	1861	1864	1869	rVB	1007871	874826	14.54%	1.924%
28	13.186	1883	1887	1891	rVB	4856734	4211210	69.99%	9.260%
29	13.263	1896	1900	1904	rBV3	60405	102509	1.70%	0.225%
30	13.374	1917	1919	1922	rVB	129893	113999	1.89%	0.251%
31	13.445	1928	1931	1933	rBV	148138	116866	1.94%	0.257%
32	13.480	1933	1937	1940	rBV2	79777	87729	1.46%	0.193%
33	14.074	2035	2038	2049	rVB4	287054	473752	7.87%	1.042%
34	14.251	2063	2068	2071	rBV2	1712306	1930704	32.09%	4.245%
35	14.274	2071	2072	2078	rVB	429009	350747	5.83%	0.771%
36	14.357	2084	2086	2089	rBV	100292	73029	1.21%	0.161%

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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	14.704	2142	2145	2146	rBV	120917	125284	2.08%	0.275%
38	15.198	2227	2229	2233	rVB	107411	112379	1.87%	0.247%
39	15.351	2251	2255	2258	rBV	318581	491114	8.16%	1.080%
40	15.409	2262	2265	2269	rVB	148426	171944	2.86%	0.378%
41	15.686	2309	2312	2318	rVB	175054	218044	3.62%	0.479%
42	15.757	2320	2324	2331	rVB	267575	378512	6.29%	0.832%
43	15.827	2331	2336	2340	rBV	920265	1179494	19.60%	2.594%
44	16.327	2417	2421	2429	rVB	141251	225721	3.75%	0.496%
45	17.456	2610	2613	2623	rVB2	88407	178373	2.96%	0.392%

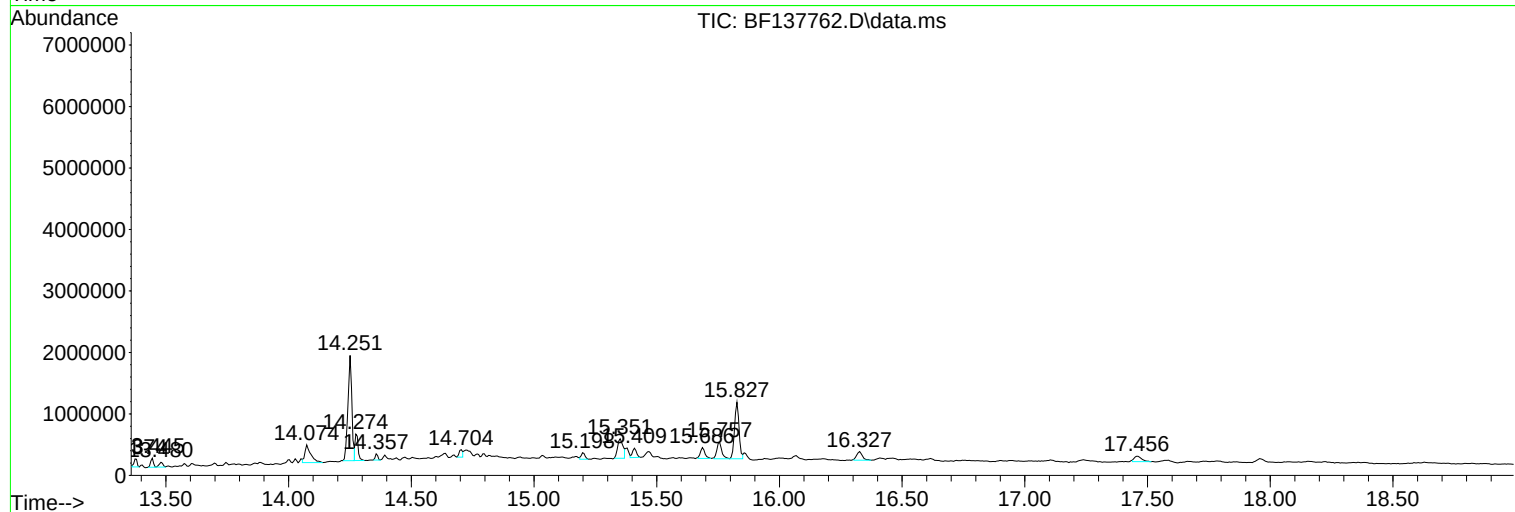
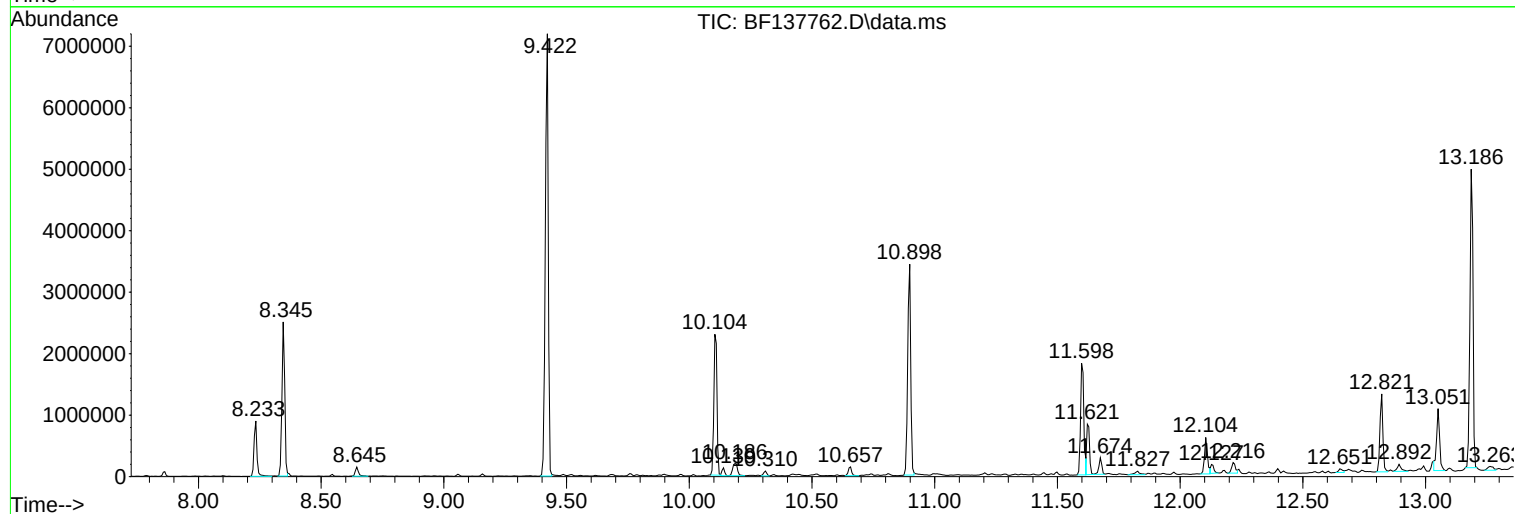
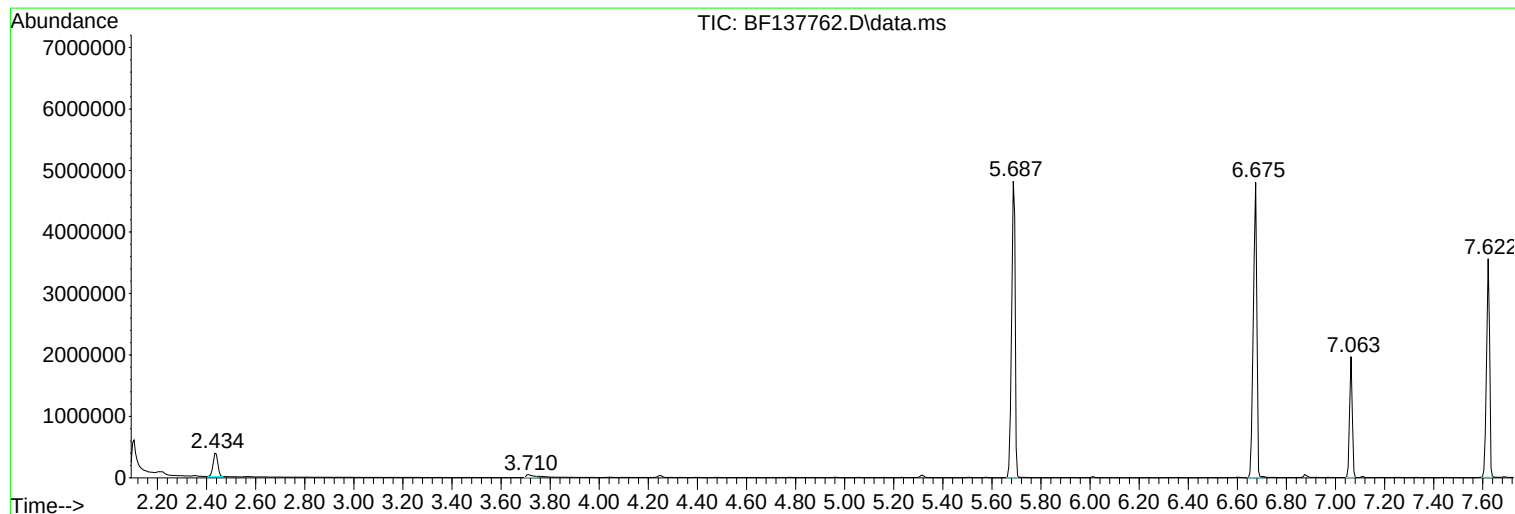
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 18 Sample Multiplier: 1

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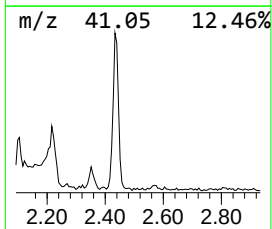
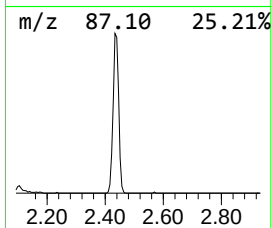
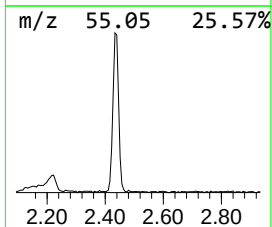
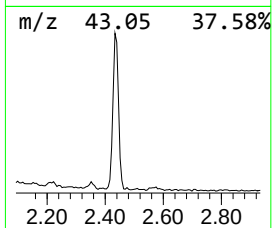
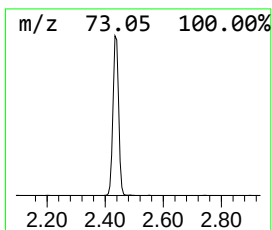
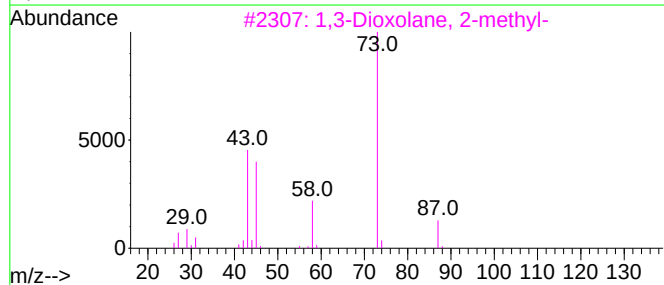
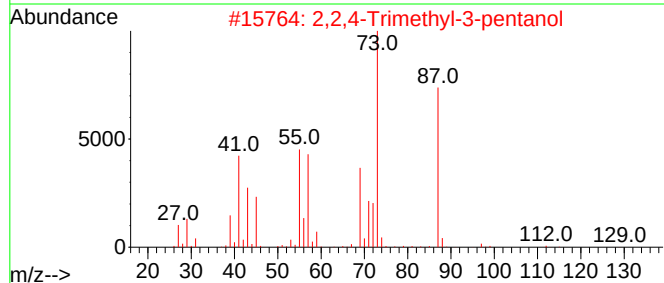
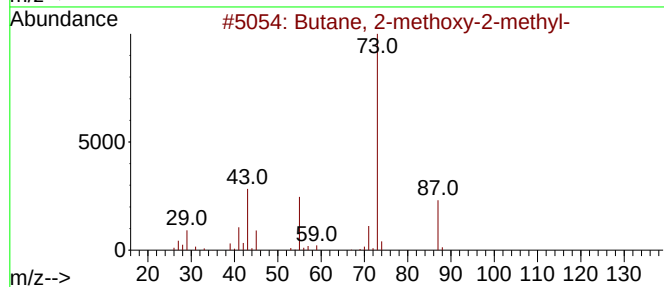
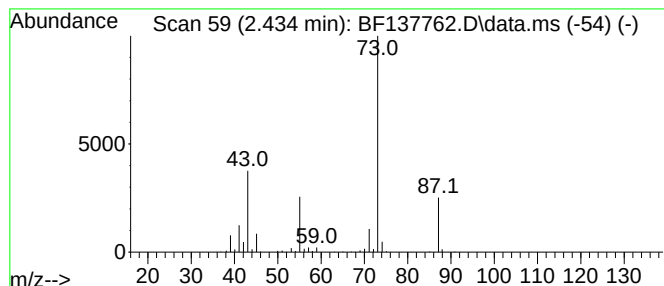
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.434	6.79 ng	512236	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		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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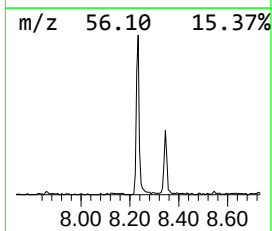
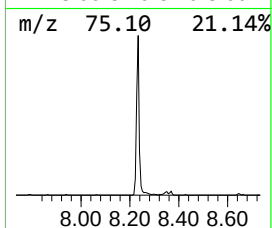
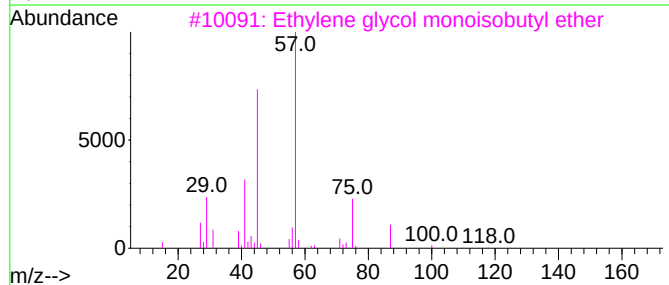
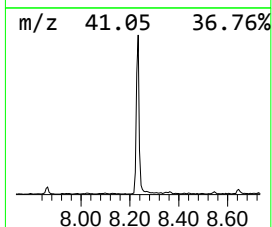
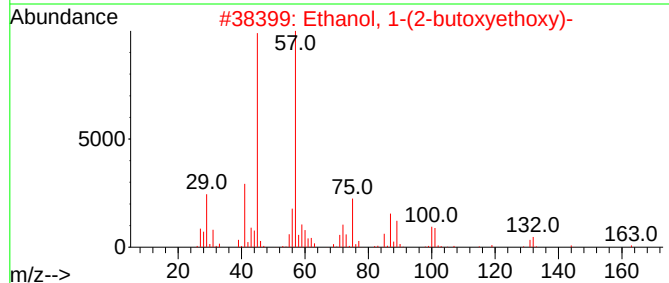
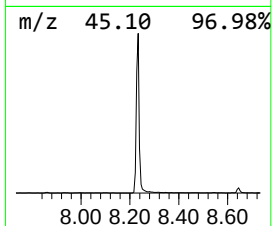
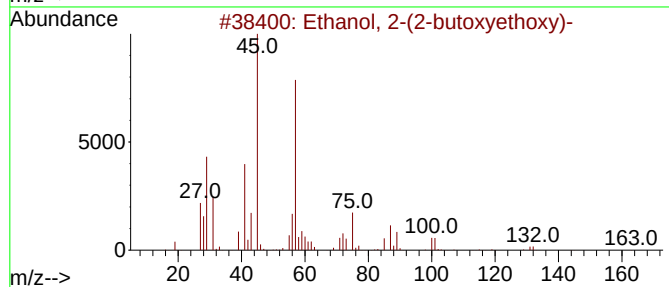
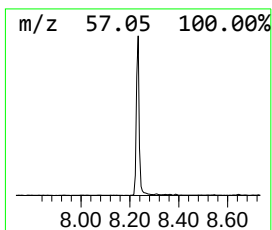
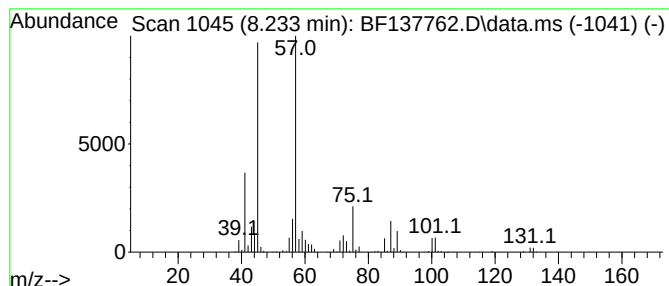
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.233	7.38 ng	735152	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	90
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		2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	50



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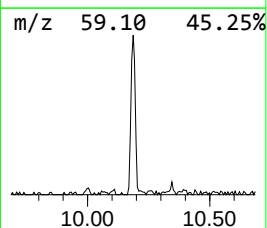
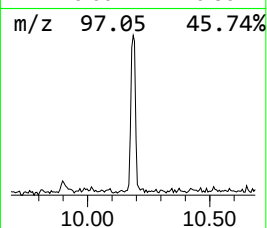
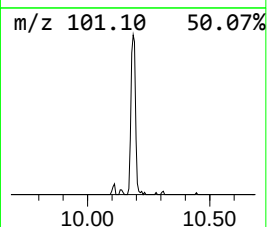
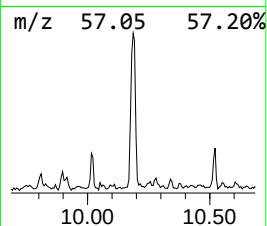
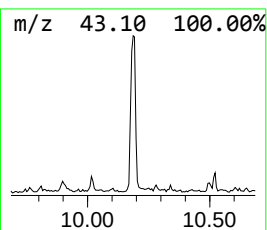
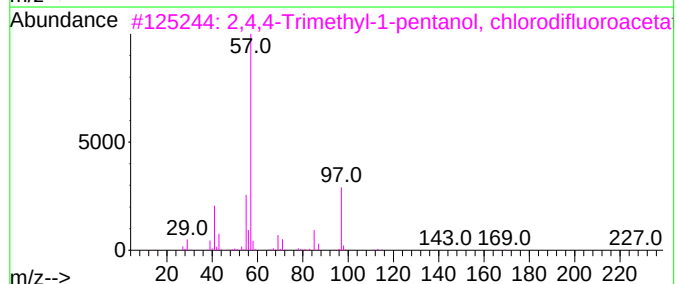
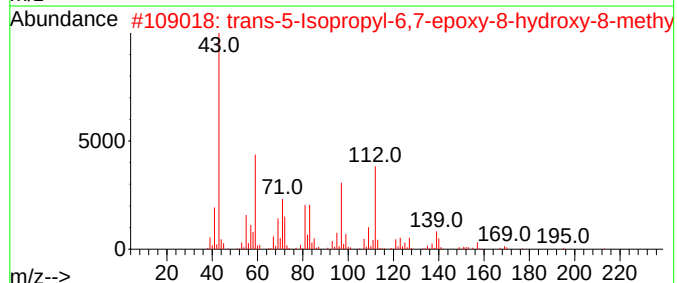
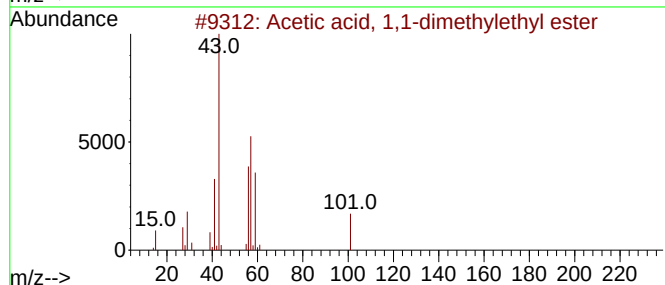
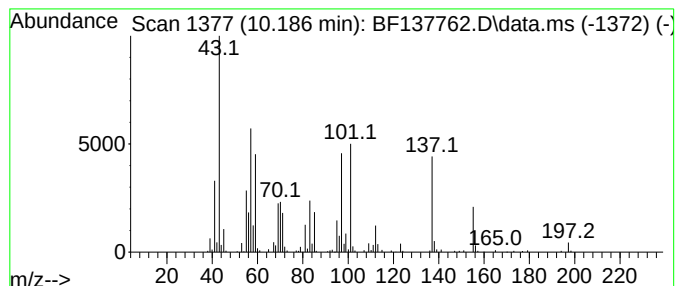
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown10.186 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.186	2.70 ng	274993	Acenaphthene-d10	10.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
2			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	10
3			2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10
4			Decane, 1-(ethenyloxy)-	184	C12H24O	000765-05-9	10
5			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10



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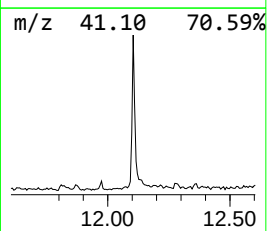
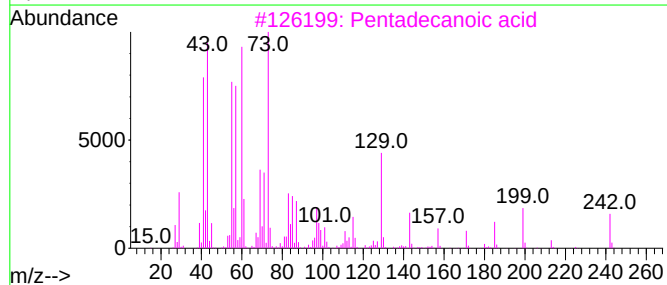
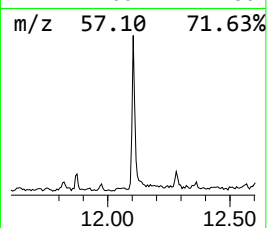
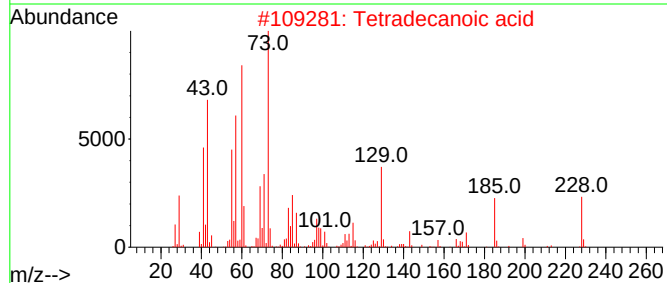
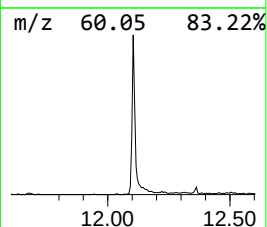
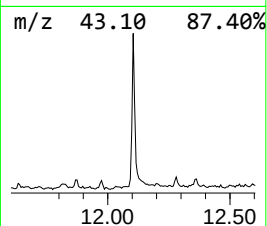
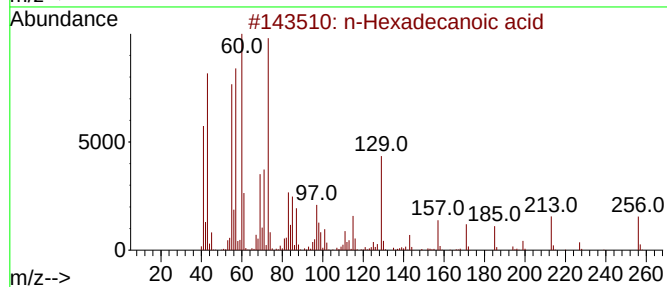
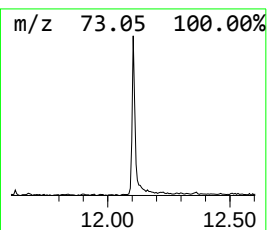
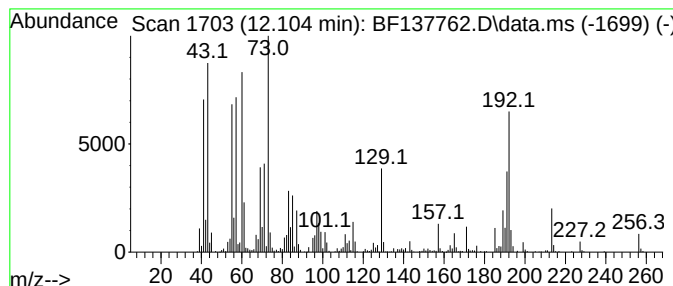
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	6.00 ng	512348	Phenanthrene-d10	11.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	59



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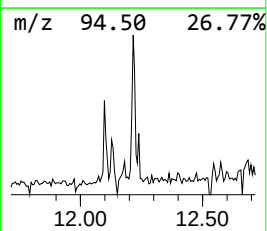
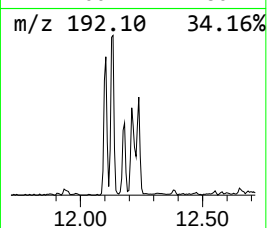
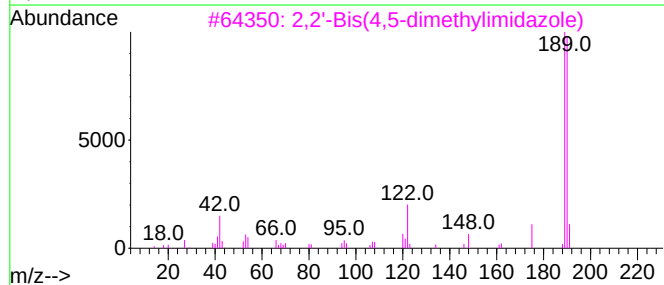
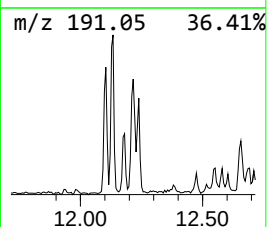
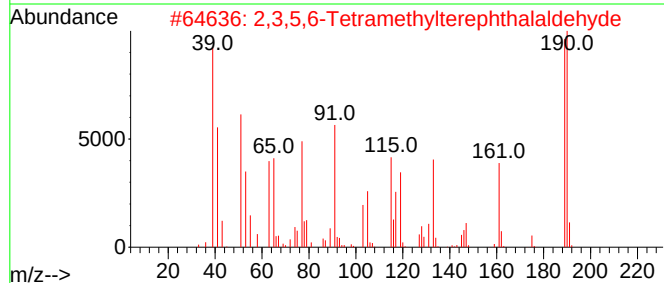
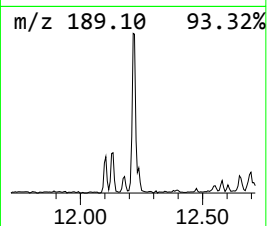
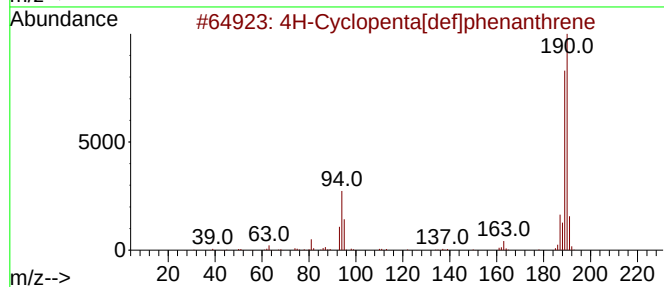
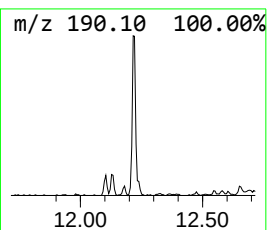
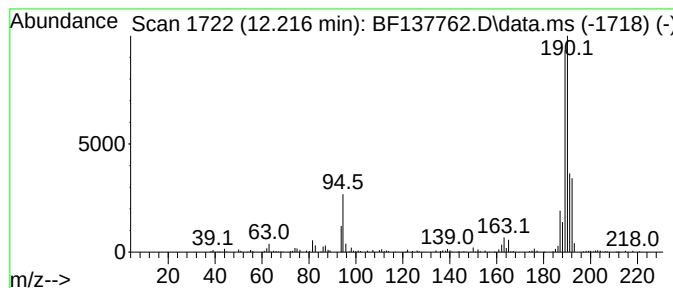
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.216	2.25 ng	191676	Phenanthrene-d10	11.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4			1,1'-Biphenyl, 4,4'-difluoro-	190	C12H8F2	000398-23-2	23
5			1-(Phenylethynyl)-1H-1,2,3-benzo...	219	C14H9N3	209912-23-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137762.D
Acq On : 29 Apr 2024 22:14
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

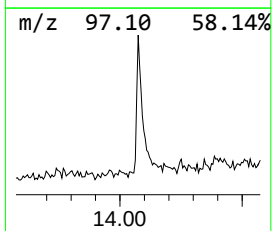
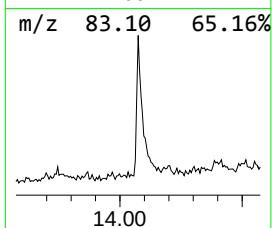
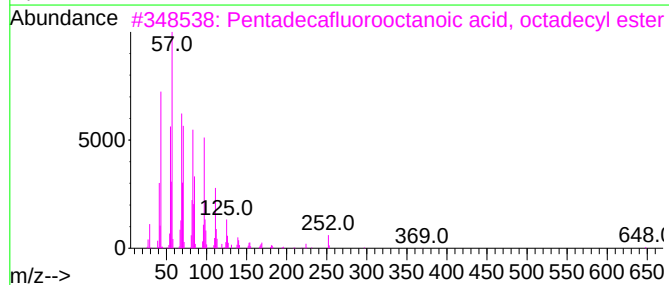
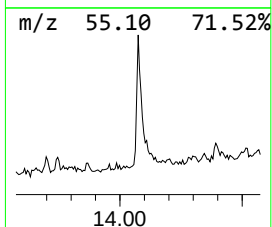
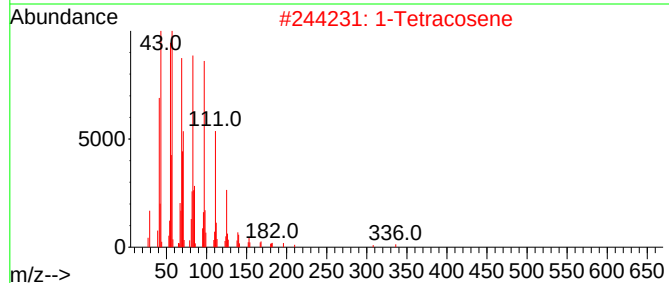
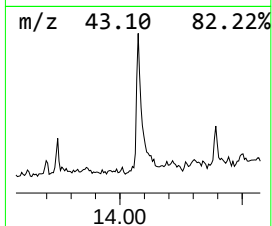
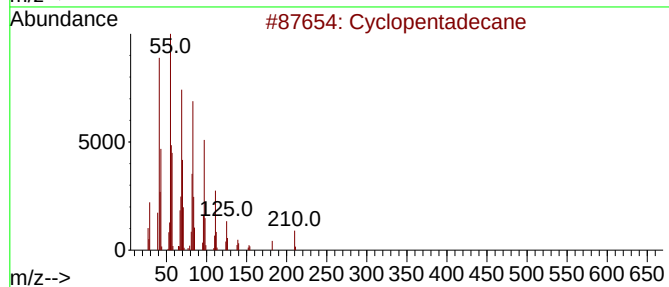
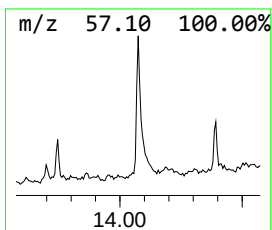
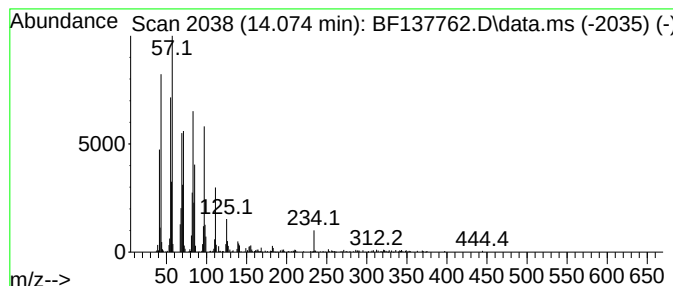
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	4.91 ng	473752	Chrysene-d12	14.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			1-Tetracosene	336	C24H48	010192-32-2	94
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4			9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
5			1-Tricosene	322	C23H46	018835-32-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137762.D
Acq On : 29 Apr 2024 22:14
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

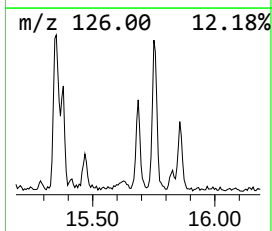
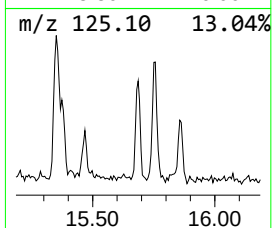
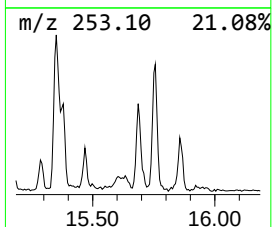
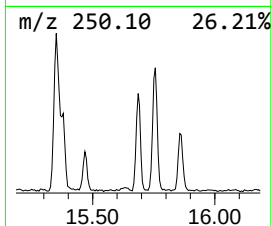
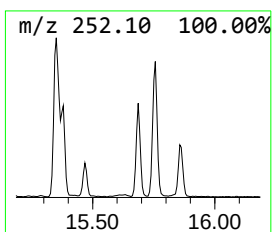
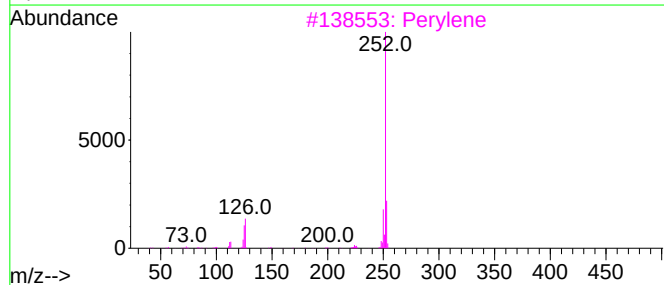
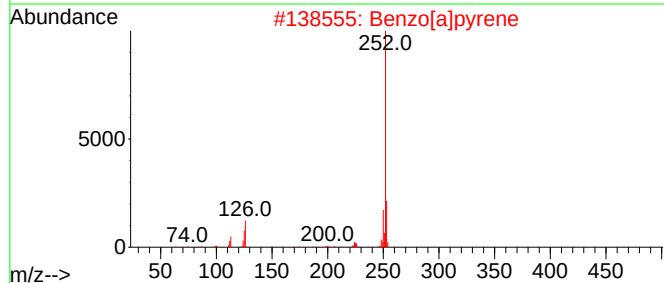
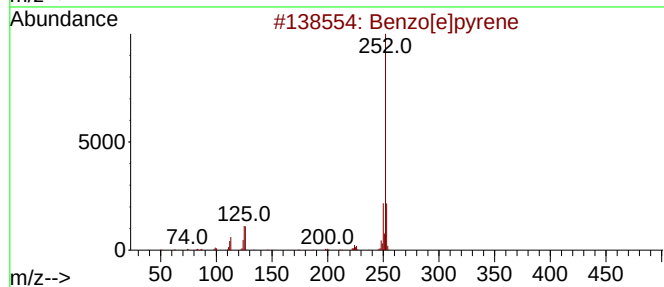
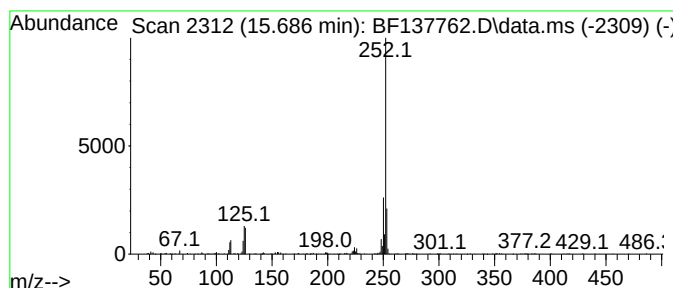
Instrument :
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ClientSampleId :
FOOT-PRINT-B-3

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 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.686	3.70 ng	218044	Perylene-d12	15.827	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[a]pyrene	252	C20H12	000050-32-8	93
3	Perylene	252	C20H12	000198-55-0	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
Data File : BF137762.D
Acq On : 29 Apr 2024 22:14
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

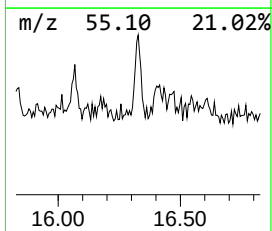
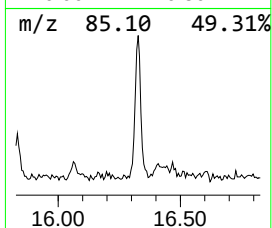
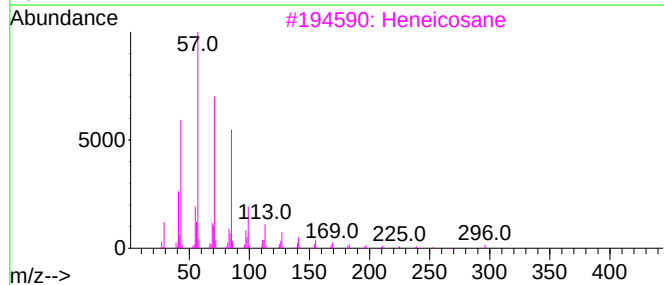
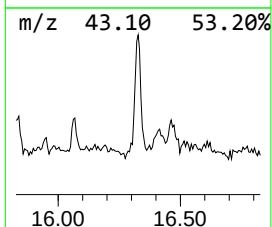
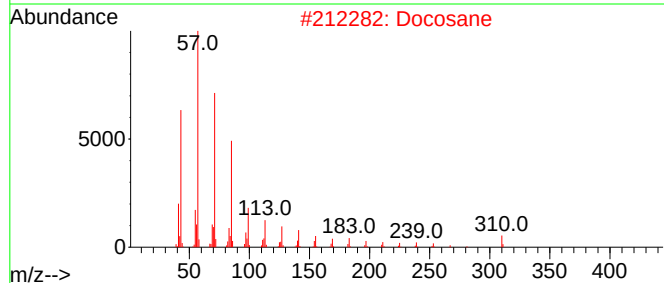
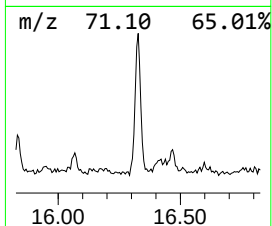
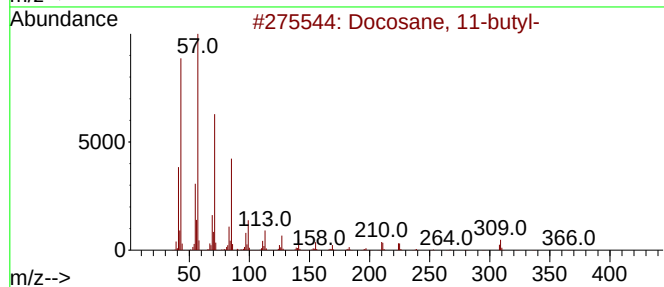
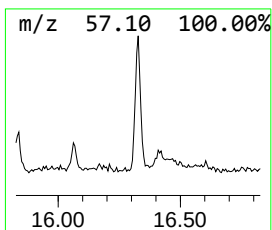
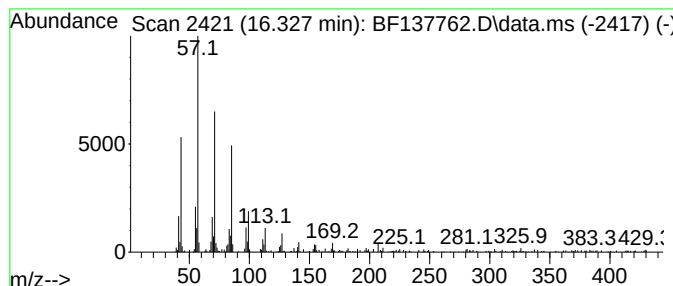
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosane, 11-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.327	3.83 ng	225721	Perylene-d12	15.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2			Docosane	310	C22H46	000629-97-0	93
3			Heneicosane	296	C21H44	000629-94-7	90
4			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042924\
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Acq On : 29 Apr 2024 22:14
Operator : CG\JU
Sample : P2294-06
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FOOT-PRINT-B-3

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.434	6.8	ng	512236	1	7.063	1508820	20.0
Ethanol, 2-(2-b...	8.233	7.4	ng	735152	2	8.345	1993560	20.0
unknown10.186	10.186	2.7	ng	274993	3	10.104	2035240	20.0
n-Hexadecanoic ...	12.104	6.0	ng	512348	4	11.598	1706930	20.0
4H-Cyclopenta[d...	12.216	2.3	ng	191676	4	11.598	1706930	20.0
Cyclopentadecane	14.074	4.9	ng	473752	5	14.251	1930700	20.0
Benzo[e]pyrene	15.686	3.7	ng	218044	6	15.827	1179490	20.0
Docosane, 11-bu...	16.327	3.8	ng	225721	6	15.827	1179490	20.0