

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
 Data File : BF139857.D
 Acq On : 18 Oct 2024 16:46
 Operator : RC/JU
 Sample : P4422-01 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EO-01-101624

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139857.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	17	rVB	692232	1077343	86.56%	6.613%
2	3.975	313	320	330	rBV	12006	21038	1.69%	0.129%
3	5.092	504	510	522	rVB	49802	72953	5.86%	0.448%
4	5.492	572	578	583	rBV	810013	1009030	81.07%	6.194%
5	6.498	743	749	759	rVV	725089	929001	74.64%	5.702%
6	6.886	810	815	821	rVB	795646	1010976	81.23%	6.206%
7	6.945	821	825	829	rBV3	11571	14360	1.15%	0.088%
8	7.286	877	883	886	rBV5	11020	17060	1.37%	0.105%
9	7.445	901	910	914	rBV	423159	555981	44.67%	3.413%
10	7.486	914	917	921	rVV	15807	22069	1.77%	0.135%
11	7.534	921	925	929	rVB4	15480	23133	1.86%	0.142%
12	7.581	929	933	939	rBV5	7442	18162	1.46%	0.111%
13	7.698	946	953	960	rVB4	37622	62342	5.01%	0.383%
14	7.769	961	965	969	rBV3	10895	20044	1.61%	0.123%
15	7.816	969	973	976	rVV3	18943	23852	1.92%	0.146%
16	7.916	987	990	996	rVB4	7294	14200	1.14%	0.087%
17	7.992	1000	1003	1008	rVB4	8909	15081	1.21%	0.093%
18	8.045	1008	1012	1015	rBV3	12123	18465	1.48%	0.113%
19	8.122	1021	1025	1027	rBV3	9503	14752	1.19%	0.091%
20	8.169	1027	1033	1040	rVV	923539	1204679	96.79%	7.395%
21	8.228	1040	1043	1046	rVV	44077	58085	4.67%	0.357%
22	8.263	1046	1049	1056	rVB7	14675	23479	1.89%	0.144%
23	8.375	1065	1068	1072	rVB3	17982	21503	1.73%	0.132%
24	8.463	1078	1083	1089	rBV7	27039	47880	3.85%	0.294%
25	8.516	1089	1092	1095	rBV5	12647	15223	1.22%	0.093%
26	8.551	1095	1098	1101	rBV3	14926	17152	1.38%	0.105%
27	8.592	1101	1105	1107	rBV	37256	46906	3.77%	0.288%
28	8.675	1116	1119	1122	rBV3	27606	33649	2.70%	0.207%
29	8.716	1123	1126	1130	rVV3	15053	22665	1.82%	0.139%
30	8.763	1130	1134	1137	rBV	40449	53151	4.27%	0.326%
31	8.922	1158	1161	1163	rBV4	15000	16097	1.29%	0.099%
32	8.951	1163	1166	1168	rBV3	15376	19563	1.57%	0.120%
33	9.169	1200	1203	1204	rBV2	17891	20241	1.63%	0.124%
34	9.192	1204	1207	1211	rVV	58892	75146	6.04%	0.461%
35	9.245	1211	1216	1220	rVB	711299	885538	71.15%	5.436%
36	9.328	1226	1230	1234	rBV	102147	140912	11.32%	0.865%

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

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37	9.639	1279	1283	1288	rBV3	106306	164255	13.20%	1.008%
38	9.792	1306	1309	1312	rBV4	32529	42930	3.45%	0.264%
39	9.851	1313	1319	1324	rVV2	68372	148643	11.94%	0.912%
40	9.922	1326	1331	1336	rVB	872531	1119023	89.91%	6.869%
41	10.357	1402	1405	1408	rVB	60183	70709	5.68%	0.434%
42	10.574	1438	1442	1448	rVB	52832	76596	6.15%	0.470%
43	10.633	1448	1452	1456	rVB	56069	66180	5.32%	0.406%
44	10.704	1460	1464	1469	rBV	401009	508681	40.87%	3.122%
45	10.833	1482	1486	1495	rVB2	109988	199111	16.00%	1.222%
46	11.274	1558	1561	1564	rBV	61052	81924	6.58%	0.503%
47	11.310	1564	1567	1573	rVB	52477	75517	6.07%	0.464%
48	11.410	1579	1584	1591	rBV	980493	1244655	100.00%	7.640%
49	11.704	1630	1634	1638	rBV	62753	79244	6.37%	0.486%
50	11.804	1647	1651	1657	rVB	86572	108048	8.68%	0.663%
51	11.933	1669	1673	1683	rBV	184174	259556	20.85%	1.593%
52	12.110	1700	1703	1707	rBV	57048	67202	5.40%	0.412%
53	12.492	1764	1768	1770	rBV	334825	483164	38.82%	2.966%
54	12.598	1783	1786	1787	rBV	41788	43573	3.50%	0.267%
55	12.645	1787	1794	1803	rVV2	350197	755021	60.66%	4.634%
56	12.721	1803	1807	1814	rVB2	87525	142215	11.43%	0.873%
57	12.851	1826	1829	1831	rBV	37084	46482	3.73%	0.285%
58	12.992	1849	1853	1861	rVB	828287	1047970	84.20%	6.433%
59	13.898	2004	2007	2017	rVB2	73724	109421	8.79%	0.672%
60	14.051	2028	2033	2044	rVB	764132	1057629	84.97%	6.492%
61	15.527	2279	2284	2289	rVB	444093	651987	52.38%	4.002%

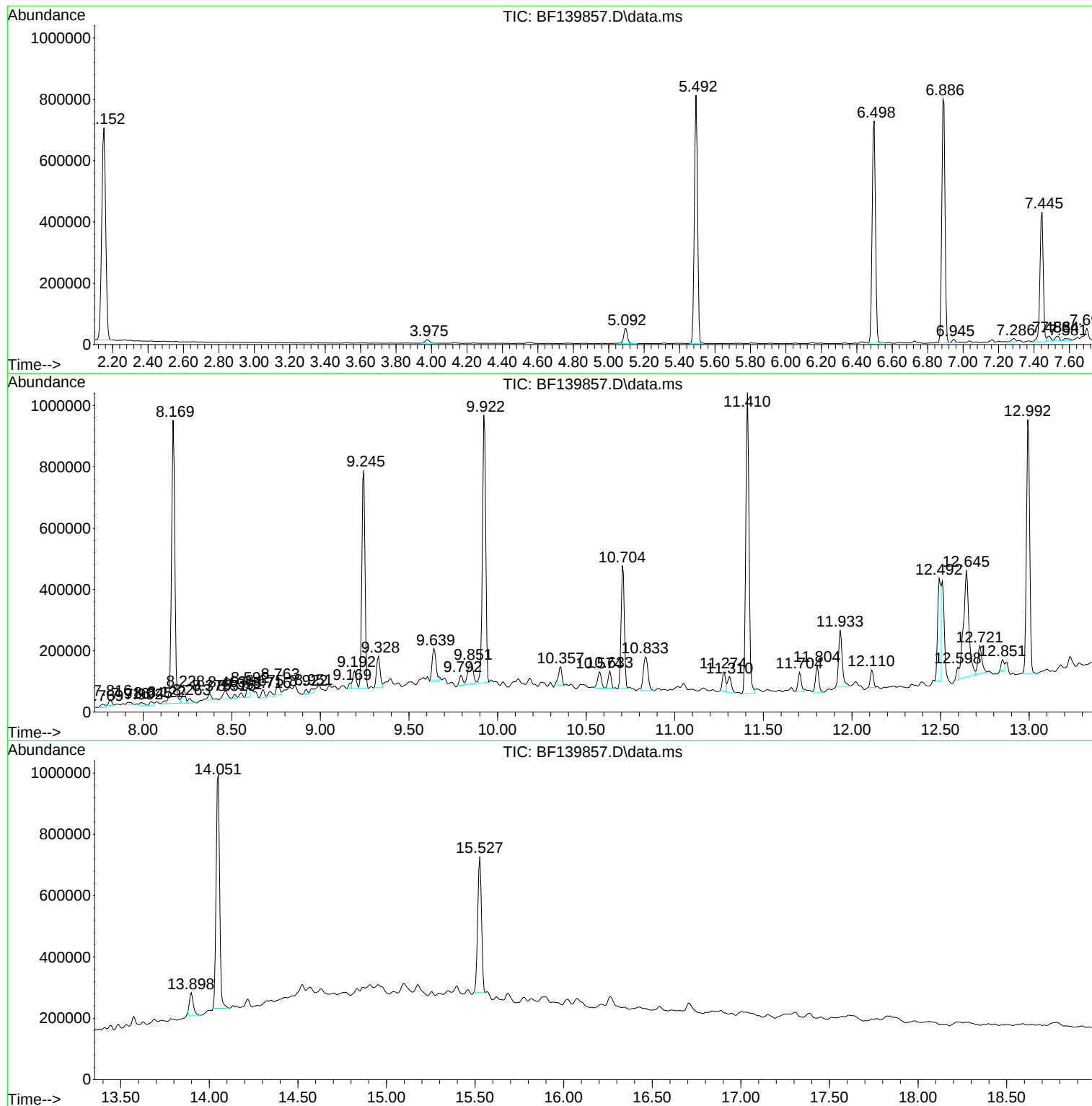
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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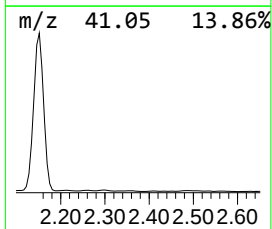
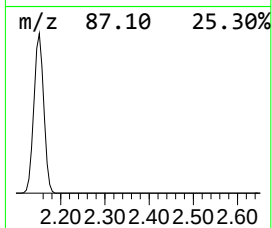
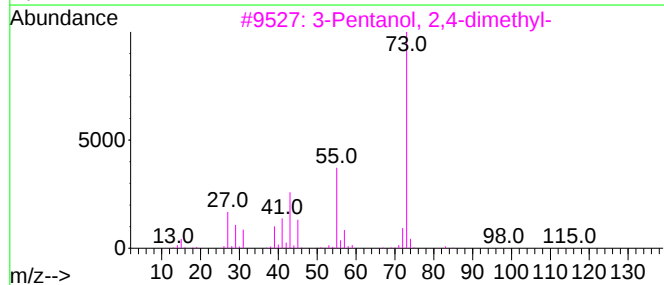
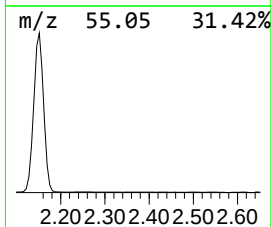
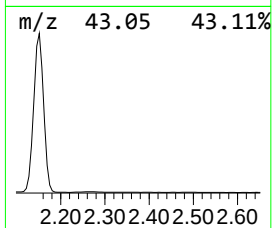
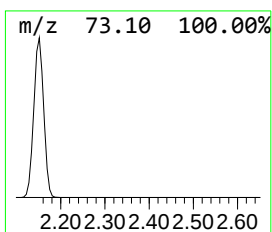
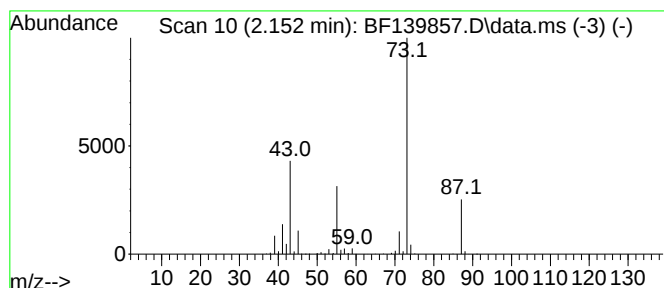
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	21.31 ng	1077340	1,4-Dichlorobenzene-d4	6.892

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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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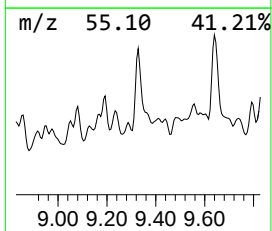
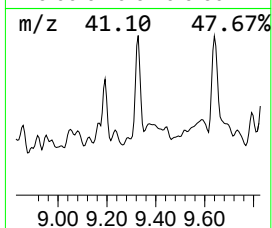
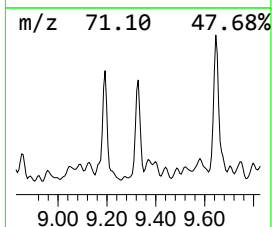
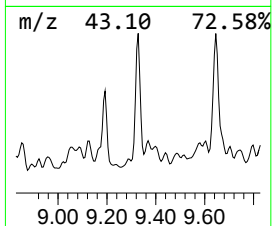
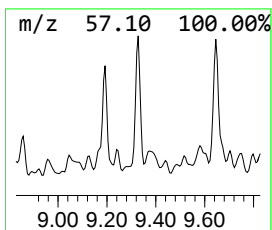
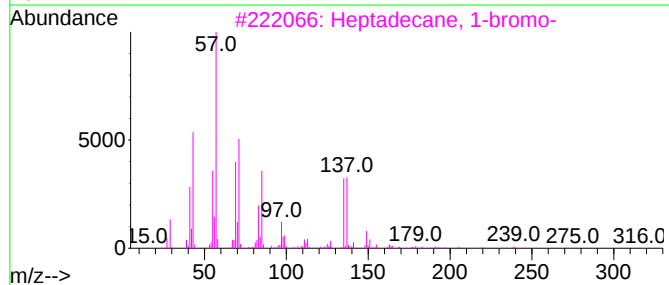
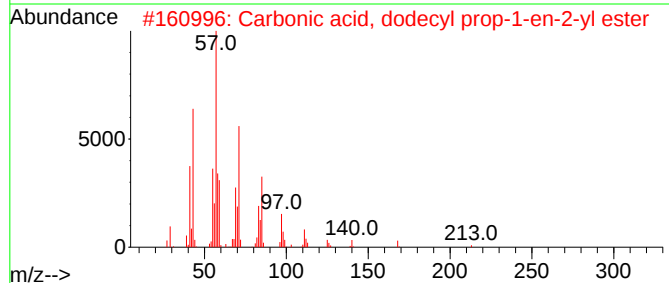
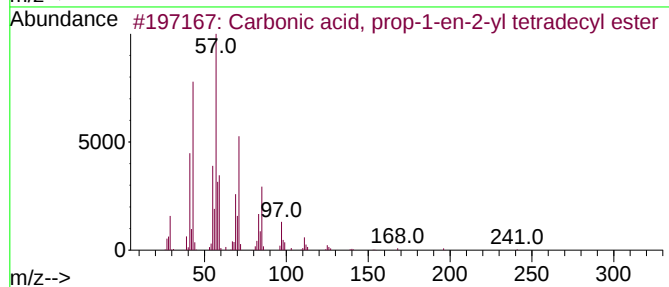
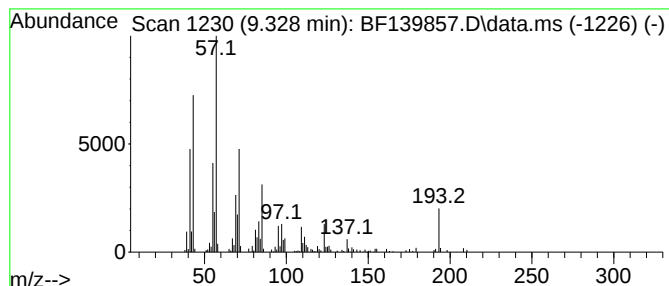
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Carbonic acid, prop-1-en-2-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.328	2.52 ng	140912	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	53
2			Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	49
3			Heptadecane, 1-bromo-	318	C17H35Br	003508-00-7	49
4			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	49
5			Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	47



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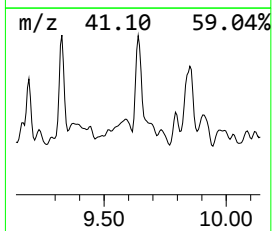
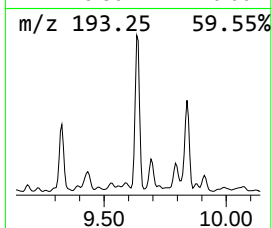
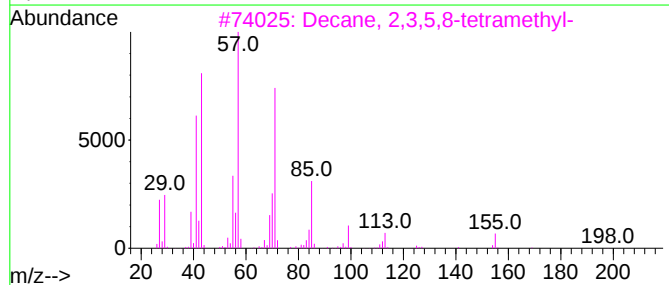
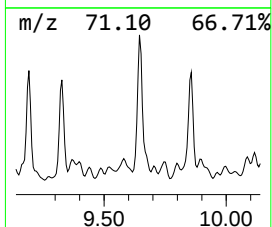
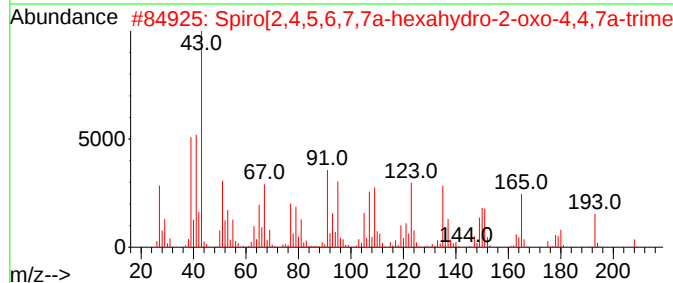
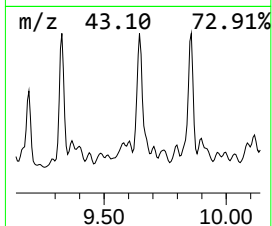
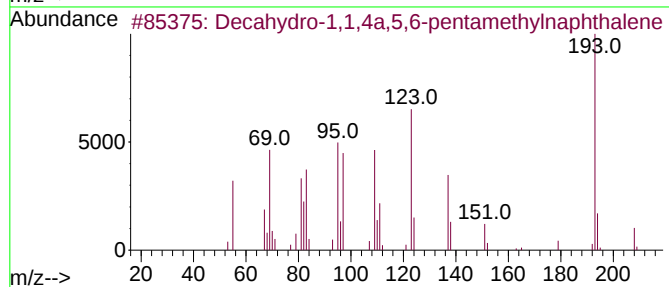
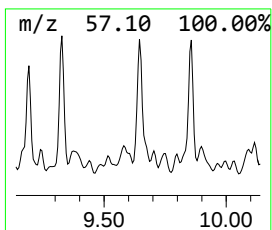
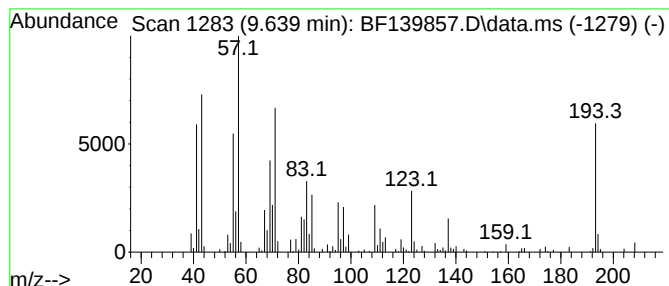
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.639	2.94 ng	164255	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	78
2			Spiro[2,4,5,6,7,7a-hexahydro-2-o...	208	C12H16O3	1000197-10-9	25
3			Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	18
4			Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	18
5			Decane, 5-propyl-	184	C13H28	017312-62-8	14



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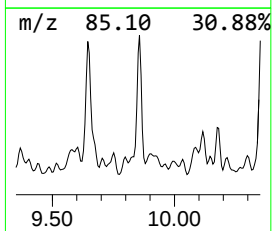
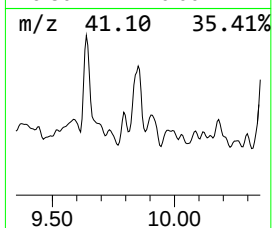
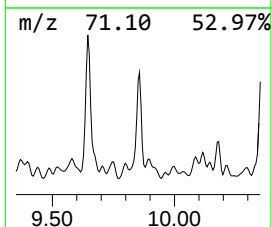
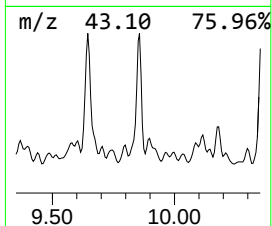
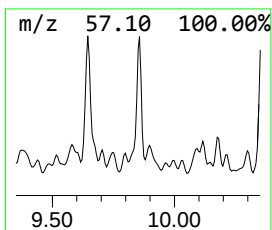
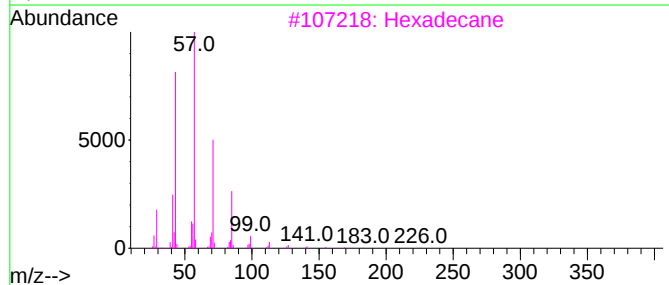
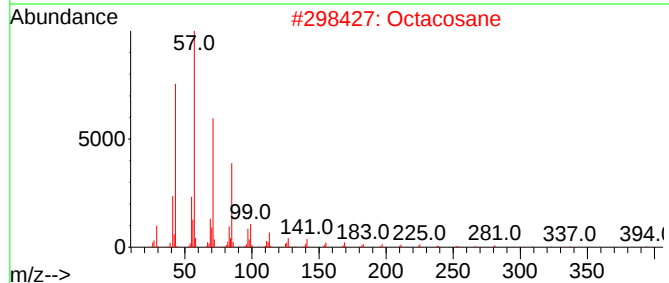
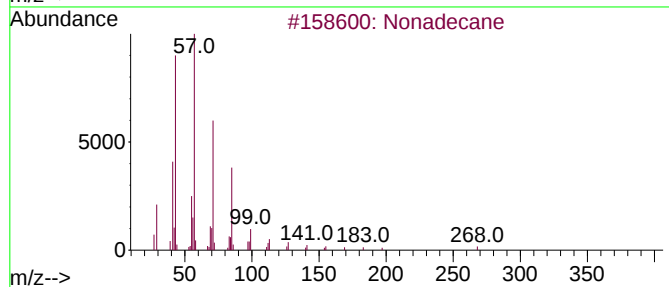
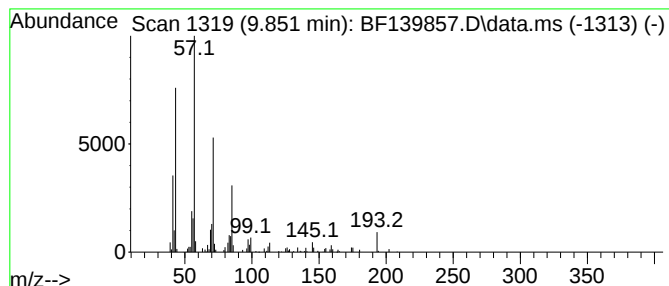
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	2.66 ng	148643	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	80
2			Octacosane	394	C28H58	000630-02-4	80
3			Hexadecane	226	C16H34	000544-76-3	80
4			Heptadecane	240	C17H36	000629-78-7	72
5			Tridecane	184	C13H28	000629-50-5	72



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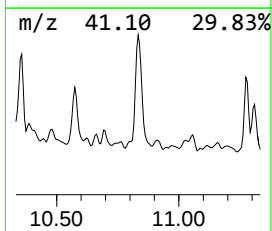
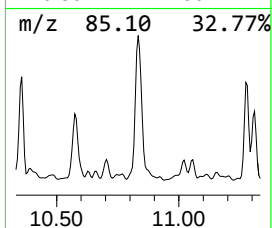
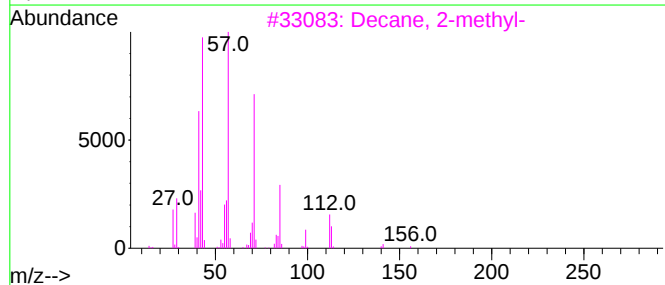
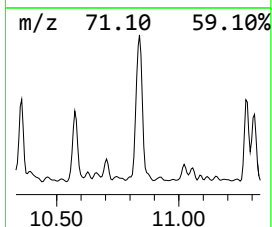
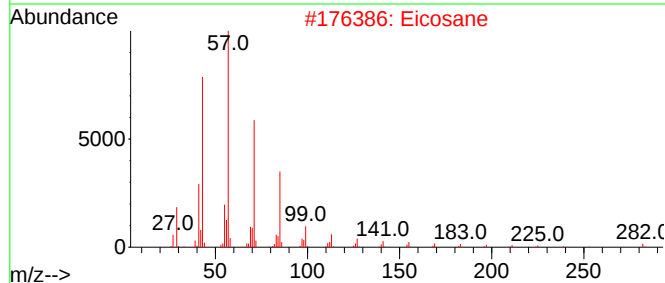
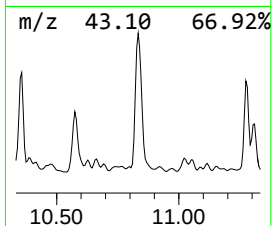
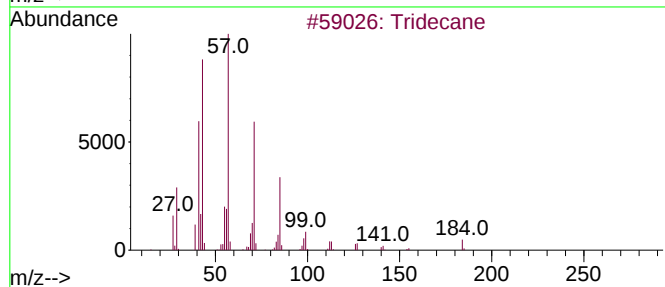
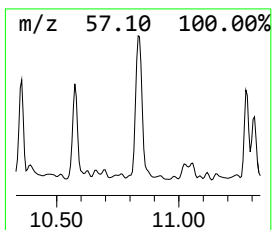
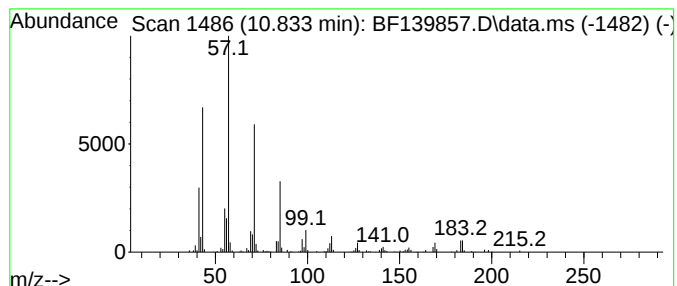
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ClientSampleId :
EO-01-101624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.833	3.20 ng	199111	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	87
2	Eicosane		282	C20H42	000112-95-8	83
3	Decane, 2-methyl-		156	C11H24	006975-98-0	81
4	Tetradecane		198	C14H30	000629-59-4	81
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139857.D
Acq On : 18 Oct 2024 16:46
Operator : RC/JU
Sample : P4422-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-01-101624

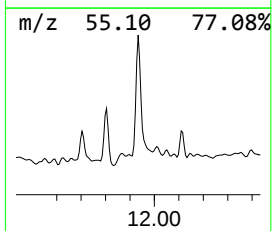
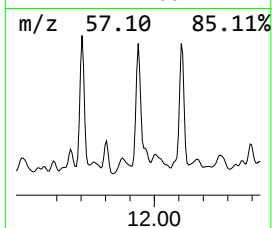
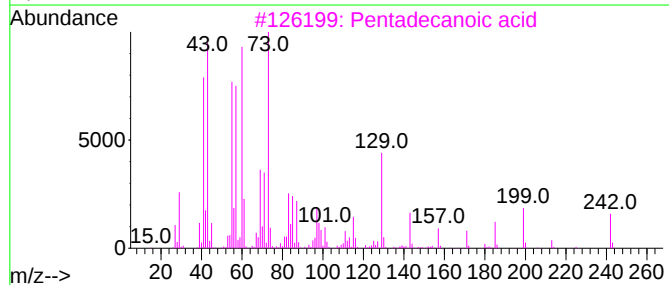
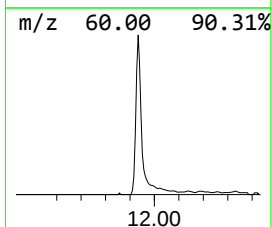
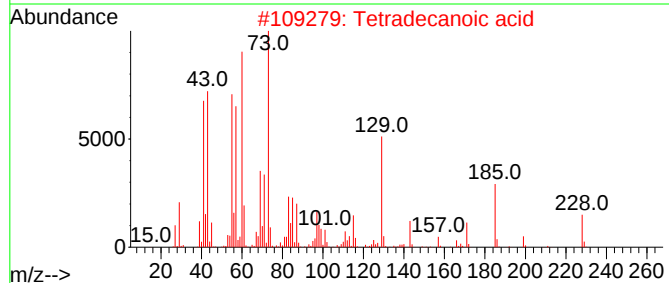
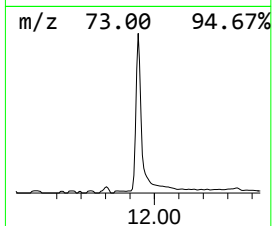
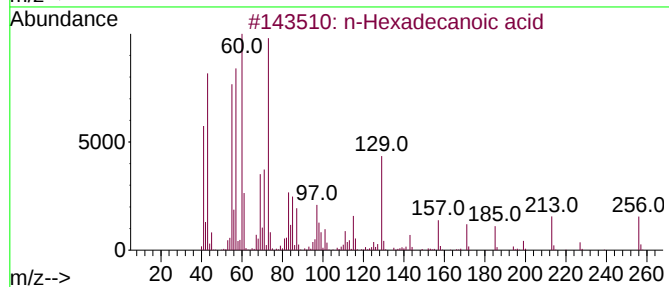
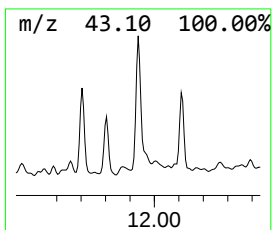
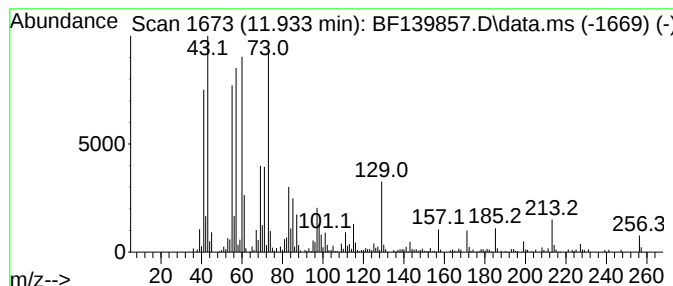
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.17 ng	259556	Phenanthrene-d10	11.410

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Octanoic acid	144	C8H16O2	000124-07-2	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139857.D
Acq On : 18 Oct 2024 16:46
Operator : RC/JU
Sample : P4422-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-01-101624

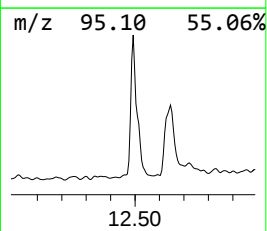
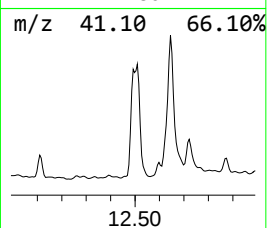
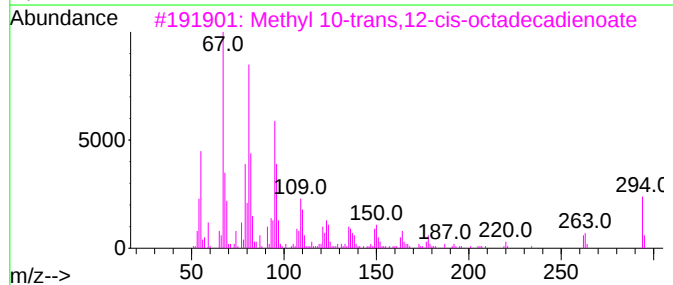
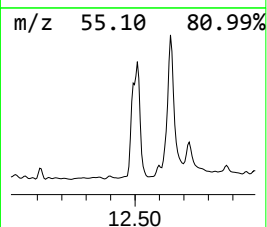
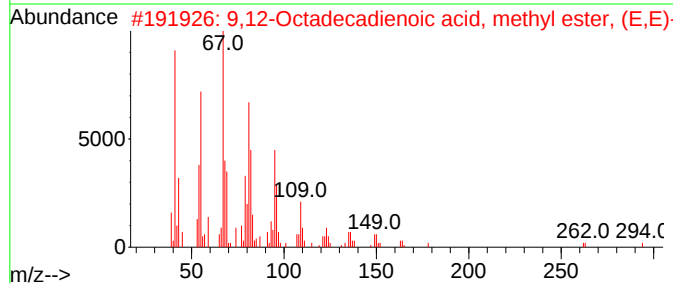
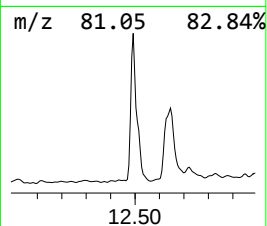
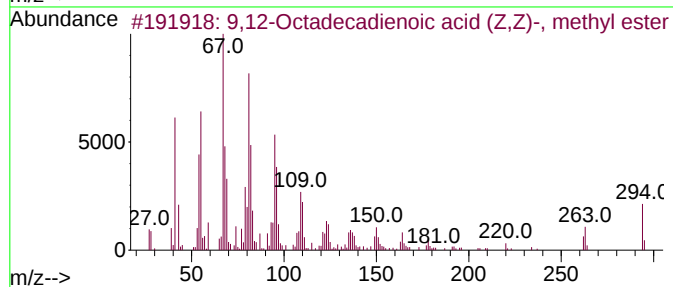
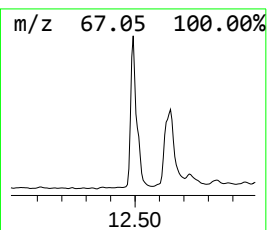
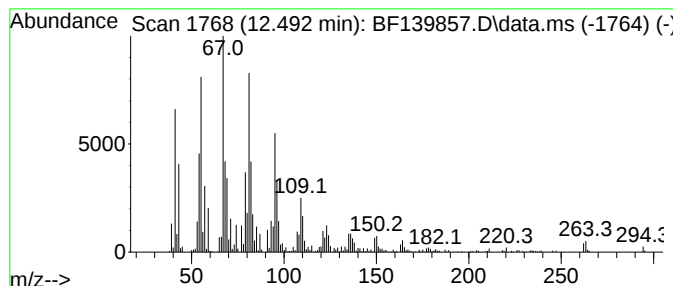
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,12-Octadecadienoic acid (... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	7.76 ng	483164	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99		
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99		
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98		
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98		
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139857.D
Acq On : 18 Oct 2024 16:46
Operator : RC/JU
Sample : P4422-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

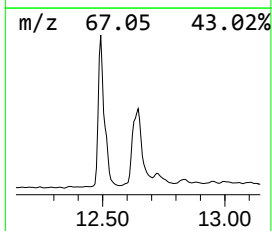
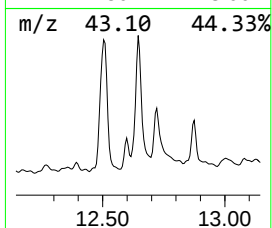
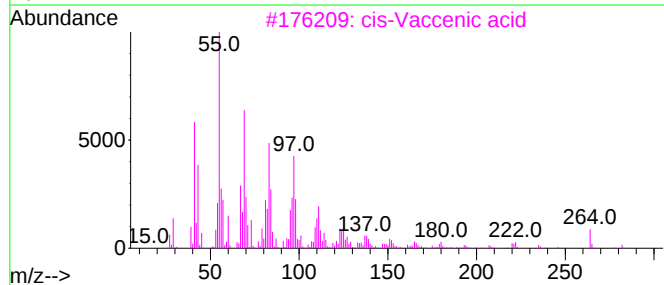
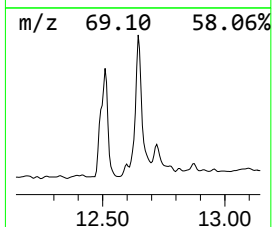
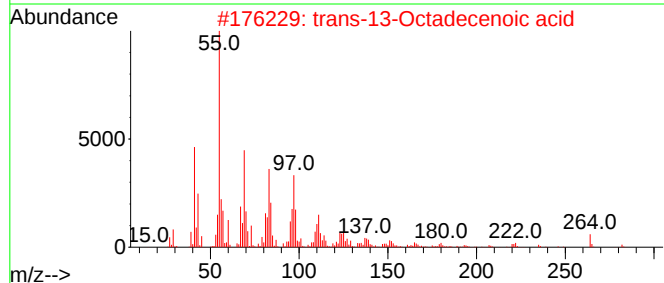
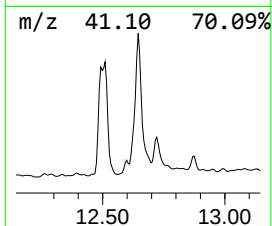
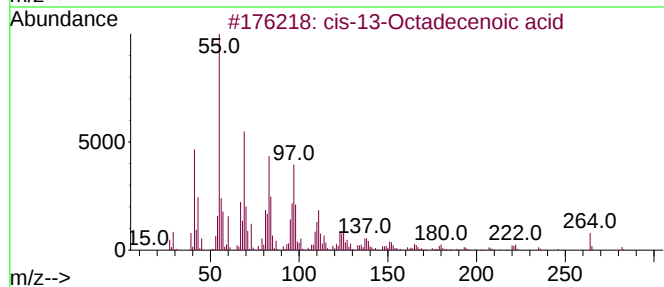
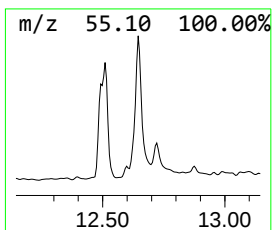
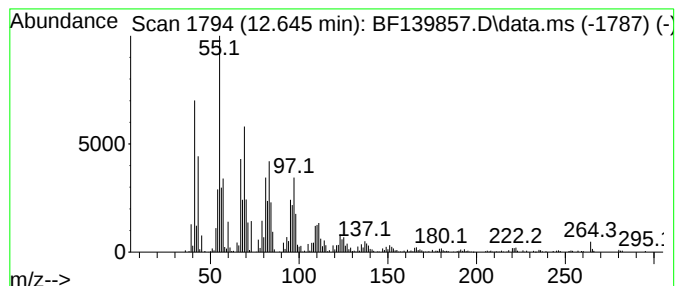
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 cis-13-Octadecenoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.645	12.13 ng	755021	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid		282	C18H34O2	013126-39-1	99
2	trans-13-Octadecenoic acid		282	C18H34O2	000693-71-0	98
3	cis-Vaccenic acid		282	C18H34O2	000506-17-2	98
4	9-Octadecenoic acid, (E)-		282	C18H34O2	000112-79-8	96
5	Palmitoleic acid		254	C16H30O2	000373-49-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139857.D
Acq On : 18 Oct 2024 16:46
Operator : RC/JU
Sample : P4422-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-01-101624

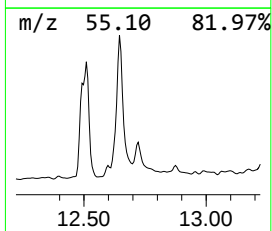
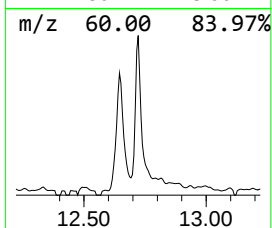
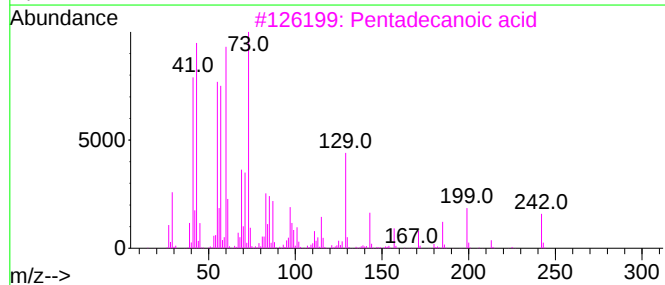
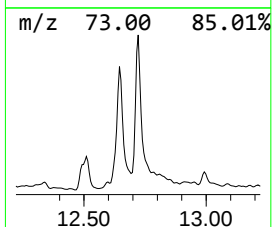
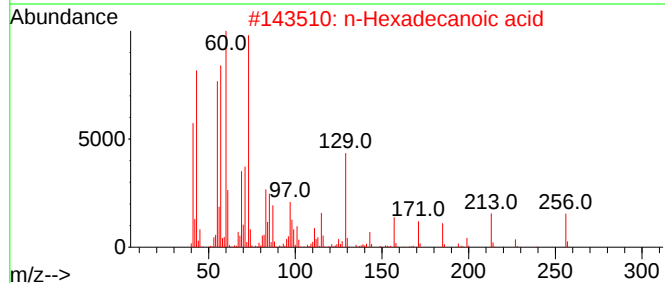
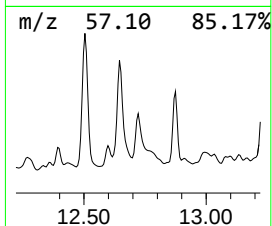
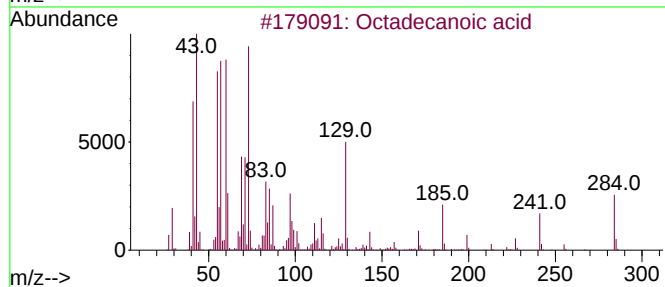
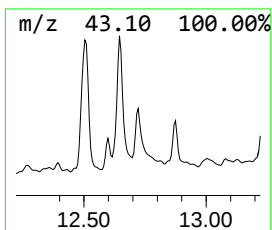
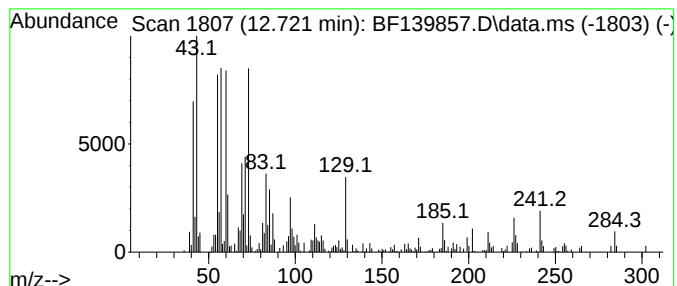
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.721	2.29 ng	142215	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139857.D
Acq On : 18 Oct 2024 16:46
Operator : RC/JU
Sample : P4422-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-01-101624

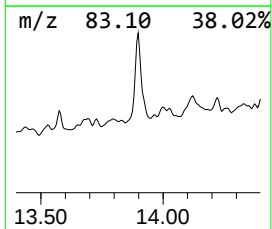
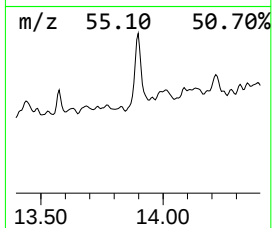
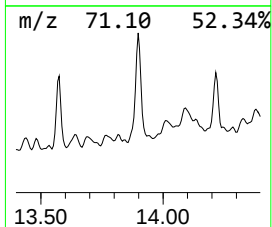
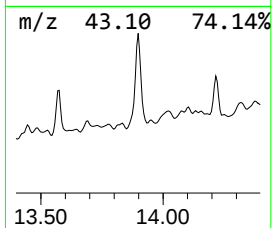
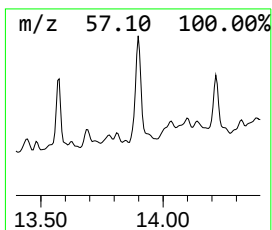
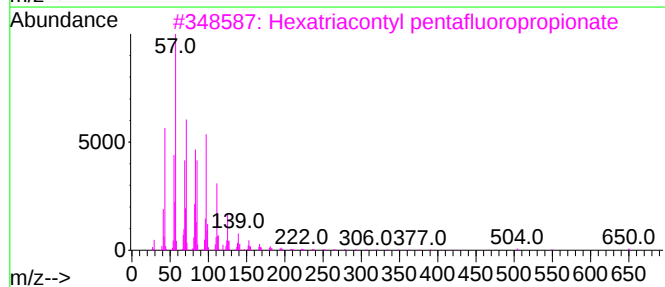
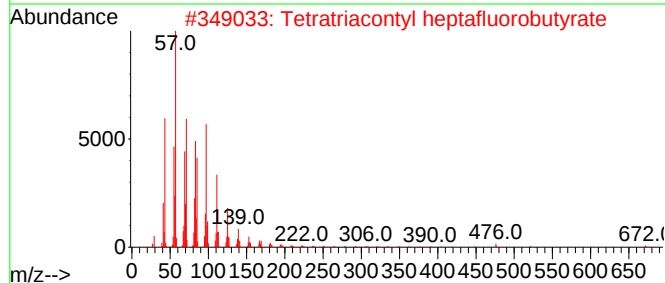
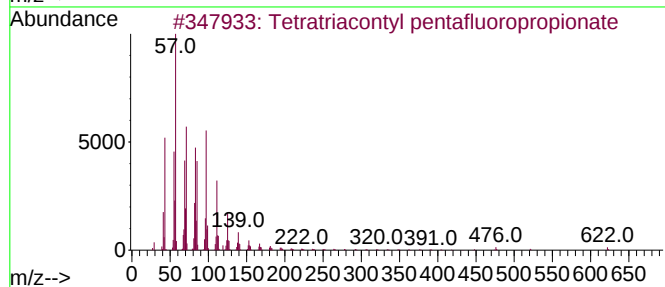
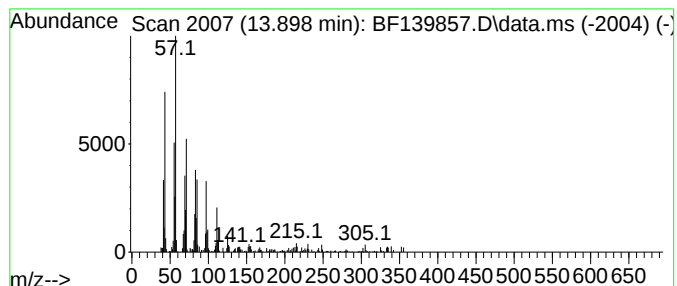
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetratriacontyl pentafluoro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.07 ng	109421	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratriacontyl pentafluoropropi...	641	C37H69F502	1000351-81-5	90
2			Tetratriacontyl heptafluorobutyrate	691	C38H69F702	1000351-84-1	90
3			Hexatriacontyl pentafluoropropio...	669	C39H73F502	1000351-89-0	90
4			1-Docosene	308	C22H44	001599-67-3	89
5			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101824\
Data File : BF139857.D
Acq On : 18 Oct 2024 16:46
Operator : RC/JU
Sample : P4422-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-01-101624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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Carbonic acid, ...	9.328	2.5	ng	140912	3	9.922	1119020	20.0
Decahydro-1,1,4...	9.639	2.9	ng	164255	3	9.922	1119020	20.0
Nonadecane	9.851	2.7	ng	148643	3	9.922	1119020	20.0
Tridecane	10.833	3.2	ng	199111	4	11.410	1244660	20.0
n-Hexadecanoic ...	11.933	4.2	ng	259556	4	11.410	1244660	20.0
9,12-Octadecadi...	12.492	7.8	ng	483164	4	11.410	1244660	20.0
cis-13-Octadece...	12.645	12.1	ng	755021	4	11.410	1244660	20.0
Octadecanoic acid	12.721	2.3	ng	142215	4	11.410	1244660	20.0
Tetratriacontyl...	13.898	2.1	ng	109421	5	14.051	1057630	20.0