

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
 Data File : BF136742.D
 Acq On : 27 Dec 2023 03:14
 Operator : CG\JU
 Sample : 05538-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-02-112223

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136742.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	494	498	508	rVB	20006	24436	1.94%	0.245%
2	5.422	563	567	581	rBV	1224531	1199624	95.46%	12.021%
3	6.428	734	738	741	rBV	1247626	1152694	91.73%	11.550%
4	6.781	795	798	802	rVB	491801	410120	32.64%	4.110%
5	7.345	889	894	897	rBV	887271	731225	58.19%	7.327%
6	7.375	897	899	902	rVB	25263	19002	1.51%	0.190%
7	7.422	902	907	910	rVB4	13007	16462	1.31%	0.165%
8	7.698	951	954	958	rVB3	15208	13602	1.08%	0.136%
9	7.816	969	974	977	rBV5	7795	13839	1.10%	0.139%
10	8.057	1009	1015	1019	rBV	557990	511590	40.71%	5.126%
11	8.122	1023	1026	1028	rVB	18054	15045	1.20%	0.151%
12	8.263	1047	1050	1052	rVB2	16528	15830	1.26%	0.159%
13	8.351	1060	1065	1067	rBV6	10228	16182	1.29%	0.162%
14	8.480	1083	1087	1089	rBV	31512	26806	2.13%	0.269%
15	8.598	1104	1107	1109	rBV2	22181	19420	1.55%	0.195%
16	8.651	1113	1116	1119	rBV	34397	27085	2.16%	0.271%
17	8.933	1162	1164	1168	rBV5	10652	13915	1.11%	0.139%
18	9.080	1187	1189	1194	rVB	38977	31268	2.49%	0.313%
19	9.139	1195	1199	1202	rBV	1407147	1256627	100.00%	12.592%
20	9.216	1208	1212	1215	rBV3	43982	41780	3.32%	0.419%
21	9.257	1215	1219	1222	rBV	67519	67592	5.38%	0.677%
22	9.539	1261	1267	1269	rBV2	39157	43549	3.47%	0.436%
23	9.751	1300	1303	1307	rVB	20220	19387	1.54%	0.194%
24	9.816	1311	1314	1317	rVB	574281	433866	34.53%	4.348%
25	10.074	1354	1358	1362	rBV6	11588	15351	1.22%	0.154%
26	10.251	1385	1388	1390	rVB	18361	16736	1.33%	0.168%
27	10.474	1421	1426	1430	rVB	22001	30238	2.41%	0.303%
28	10.610	1445	1449	1456	rBV	641889	577448	45.95%	5.786%
29	10.733	1466	1470	1477	rVB	39480	56843	4.52%	0.570%
30	11.204	1547	1550	1555	rVB	27768	28027	2.23%	0.281%
31	11.310	1564	1568	1571	rBV	487204	425606	33.87%	4.265%
32	11.604	1608	1618	1622	rBV4	20864	45500	3.62%	0.456%
33	11.704	1633	1635	1641	rVB	47088	40823	3.25%	0.409%
34	11.839	1655	1658	1667	rBV	126135	138211	11.00%	1.385%
35	12.092	1698	1701	1708	rBV	50056	48508	3.86%	0.486%
36	12.239	1723	1726	1732	rBV8	9191	18178	1.45%	0.182%

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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

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37	12.363	1744	1747	1749	rBV4	15351	17079	1.36%	0.171%
38	12.392	1749	1752	1754	rVV	224088	211705	16.85%	2.121%
39	12.415	1754	1756	1761	rVB2	161180	139206	11.08%	1.395%
40	12.504	1768	1771	1773	rBV	24973	17787	1.42%	0.178%
41	12.527	1773	1775	1777	rBV	18092	16284	1.30%	0.163%
42	12.633	1790	1793	1799	rBV5	25764	35560	2.83%	0.356%
43	12.757	1811	1814	1816	rBV	19035	18550	1.48%	0.186%
44	12.904	1835	1839	1842	rBV	1386785	1151064	91.60%	11.534%
45	13.139	1876	1879	1883	rBV4	19765	24038	1.91%	0.241%
46	13.815	1991	1994	1996	rBV3	21821	22855	1.82%	0.229%
47	13.857	1997	2001	2005	rBV7	25170	54323	4.32%	0.544%
48	13.962	2015	2019	2023	rBV	453691	400468	31.87%	4.013%
49	14.821	2162	2165	2169	rVB	76486	72716	5.79%	0.729%
50	15.445	2267	2271	2275	rBV	201710	235583	18.75%	2.361%

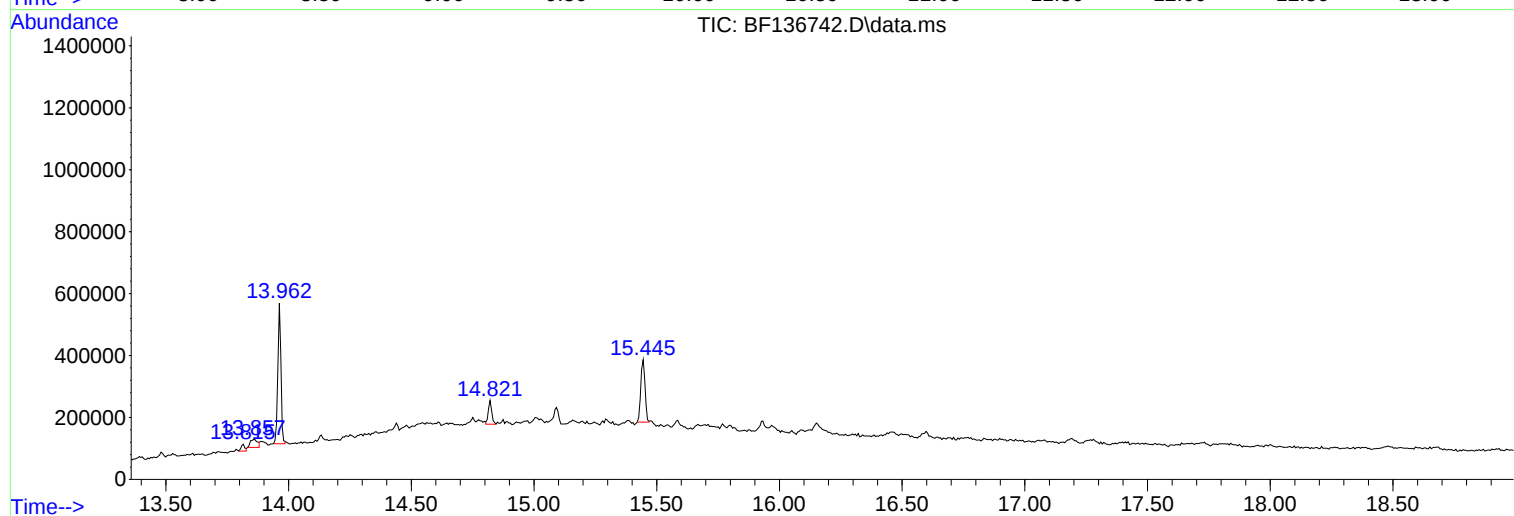
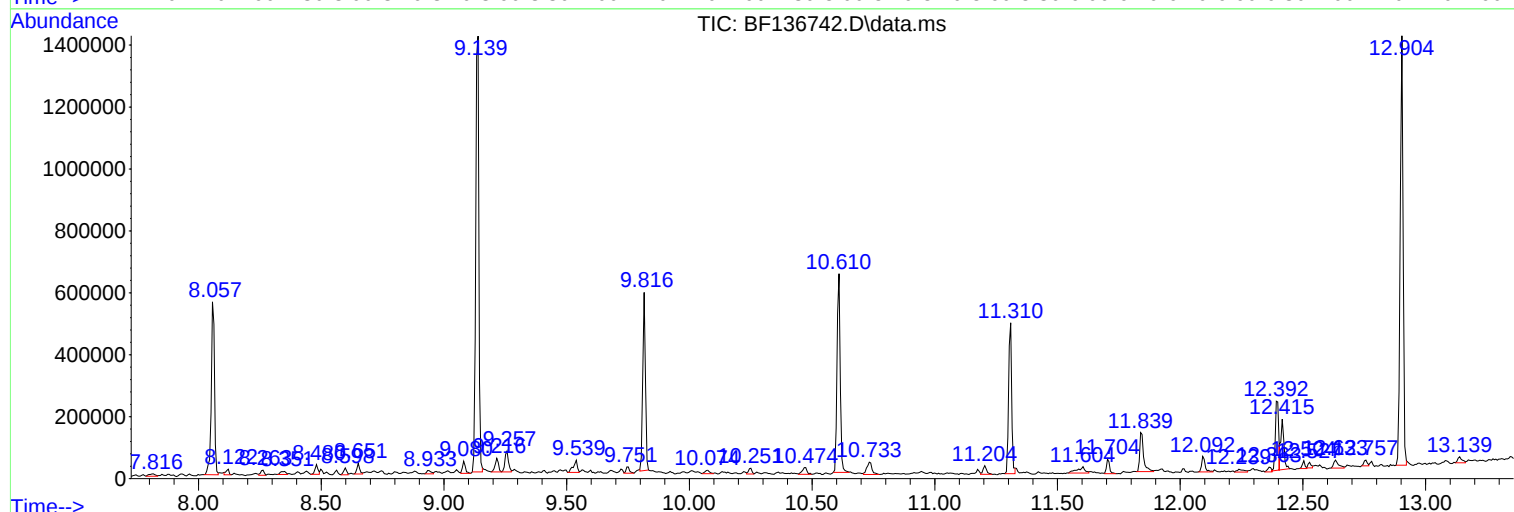
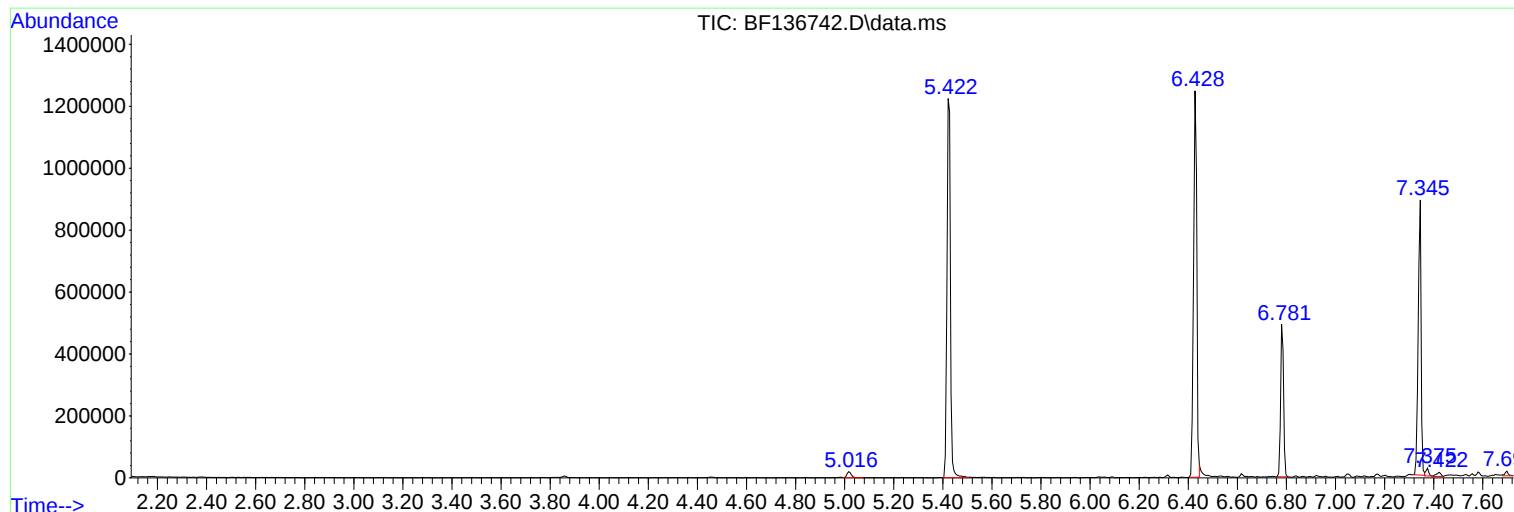
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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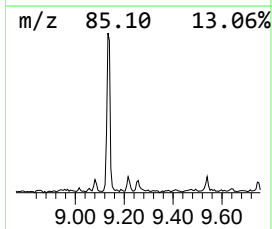
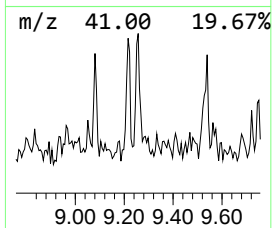
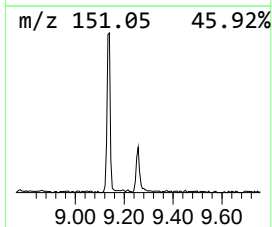
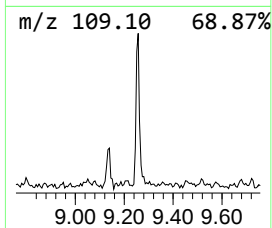
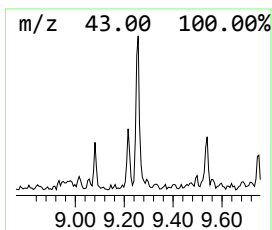
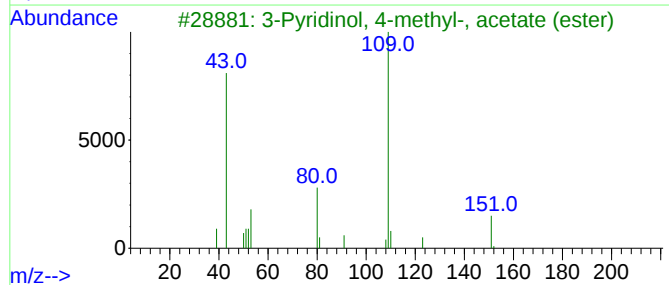
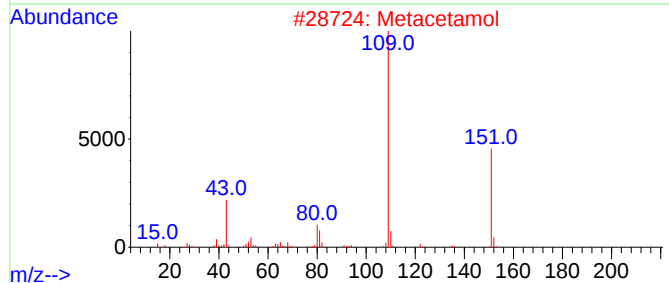
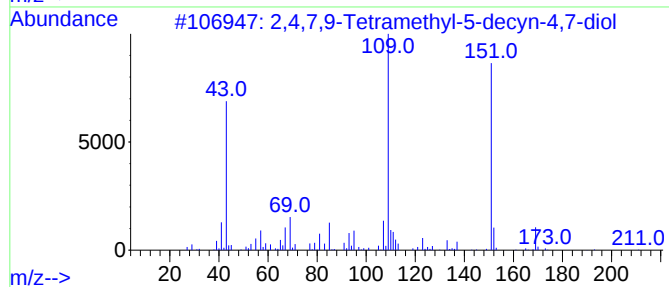
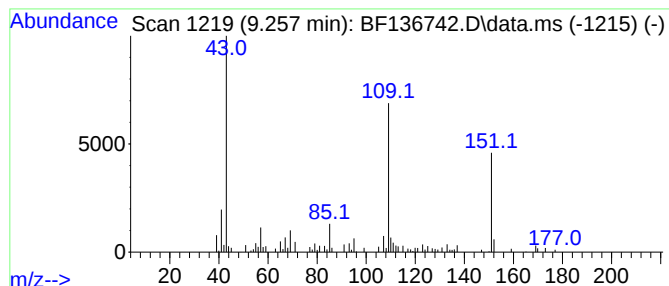
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	3.12 ng	67592	Acenaphthene-d10	9.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Metacetamol	151	C8H9NO2	000621-42-1	58	
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	58	
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53	
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	42	



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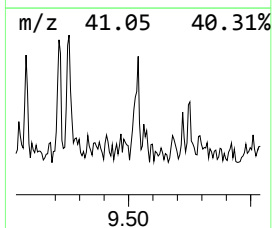
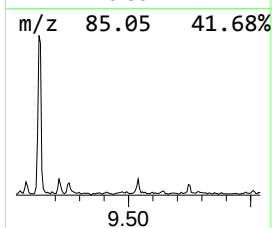
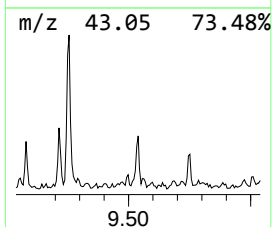
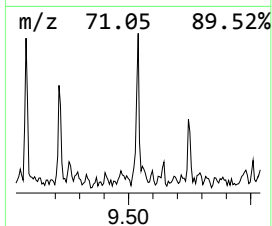
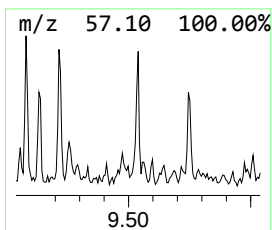
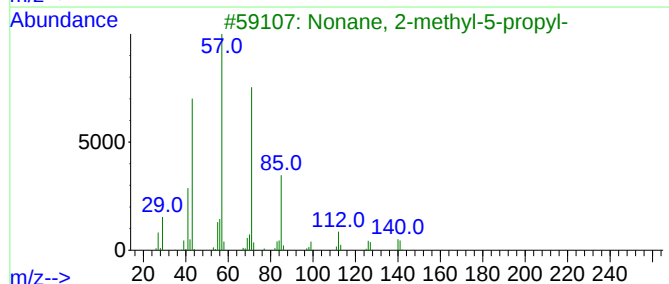
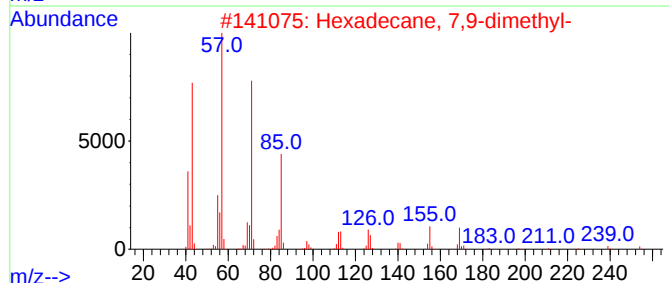
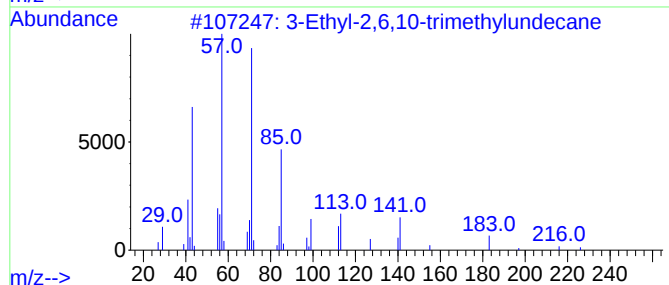
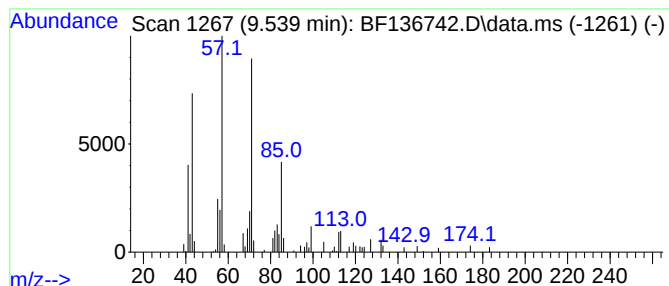
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Ethyl-2,6,10-trimethylund... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.539	2.01 ng	43549	Acenaphthene-d10	9.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	86
2		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	86
3		Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	78
4		2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	78
5		Heptadecane, 7-methyl-	254	C18H38	020959-33-5	72



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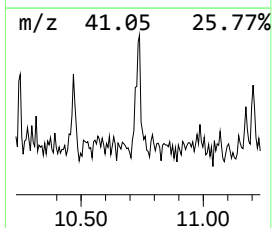
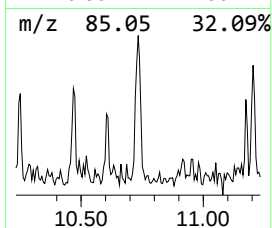
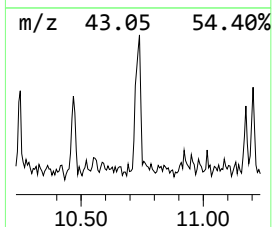
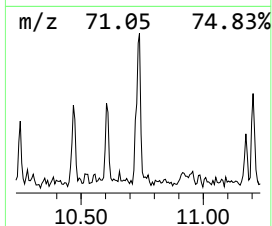
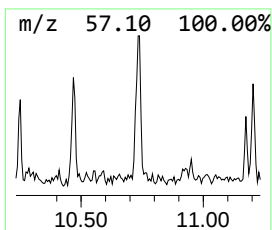
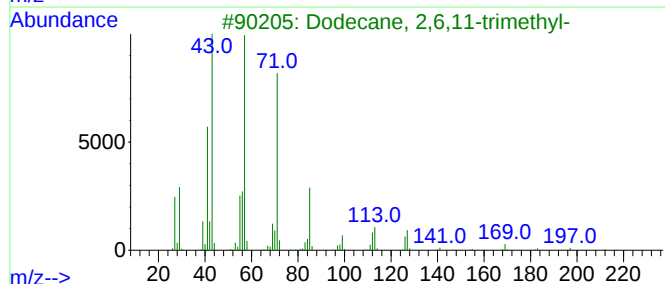
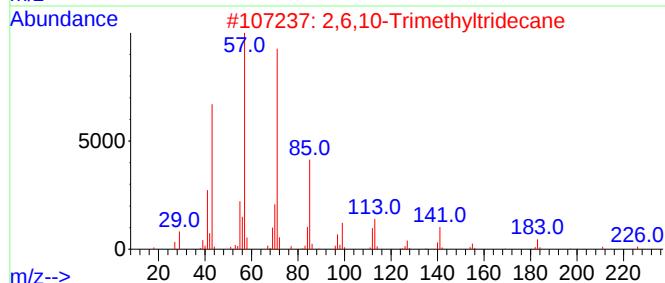
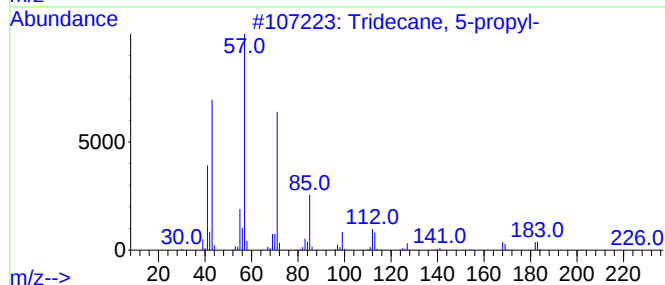
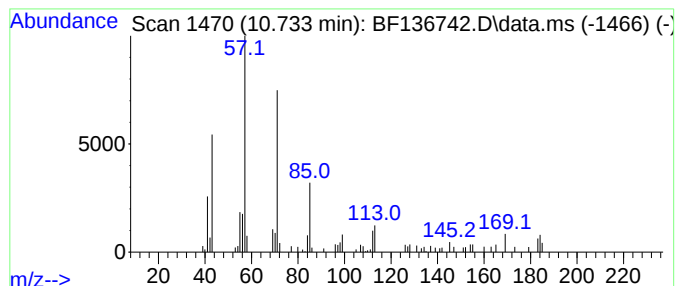
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecane, 5-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.733	2.67 ng	56843	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
2			2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	72
3			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
4			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	64
5			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	59



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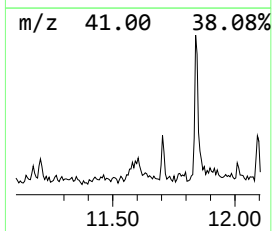
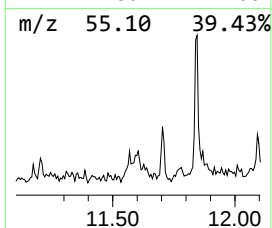
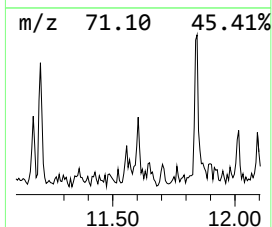
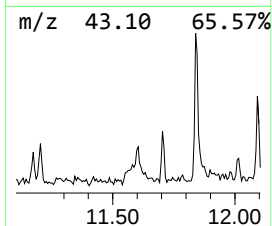
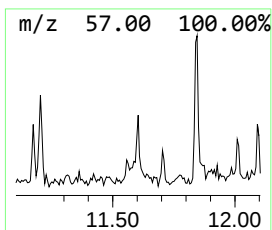
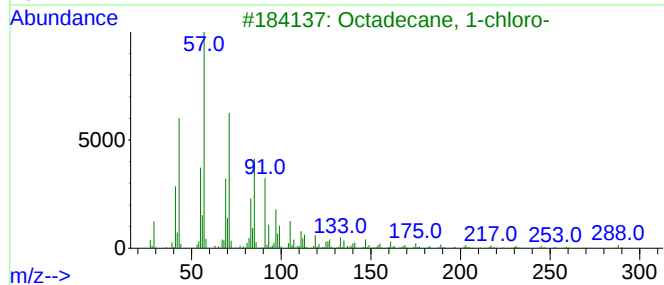
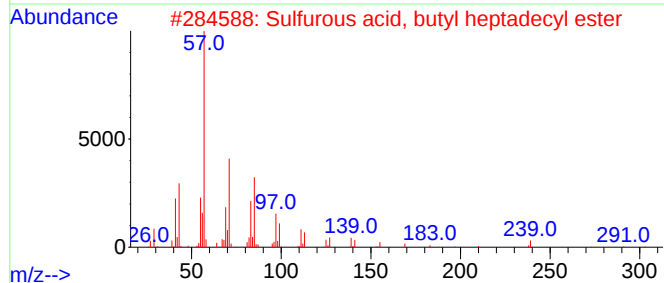
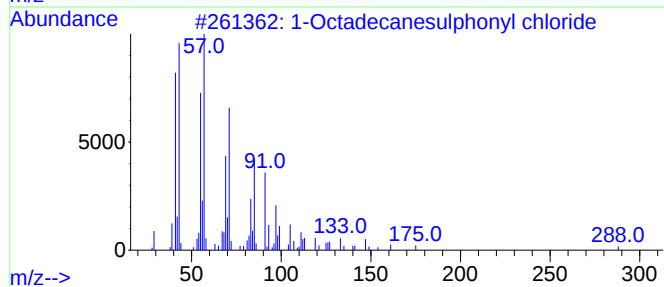
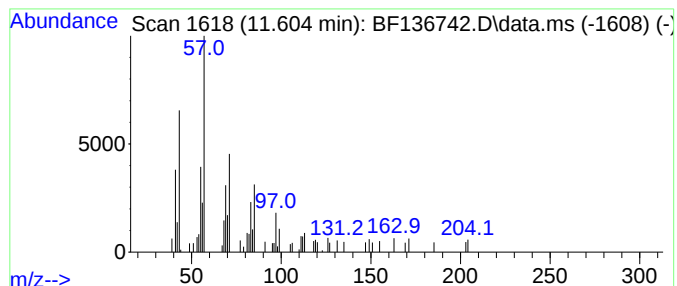
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Octadecanesulphonyl chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.604	2.14 ng	45500	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	86
2			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	80
3			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	72
4			Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	72
5			Carbonic acid, decyl undecyl ester	356	C22H44O3	1000383-16-0	64



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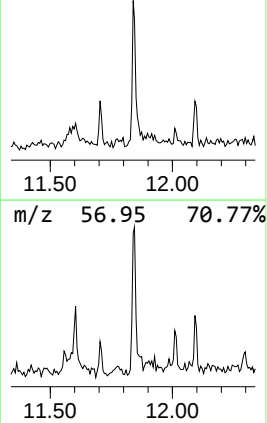
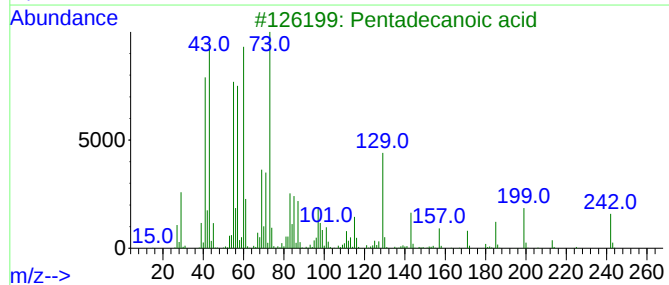
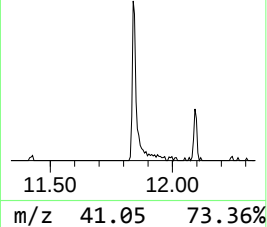
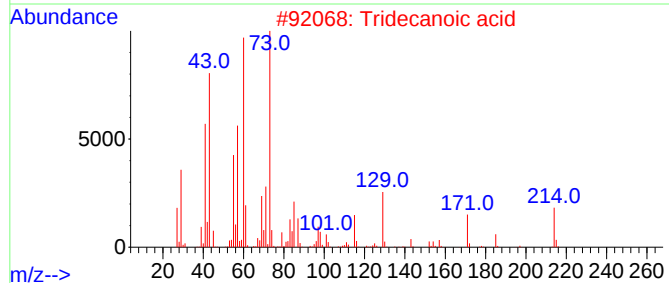
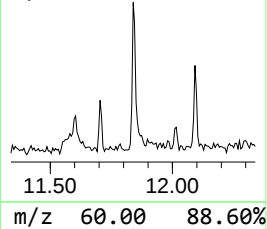
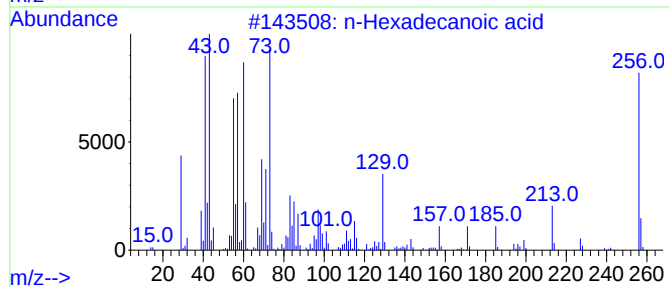
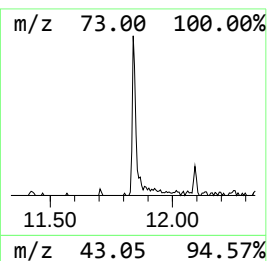
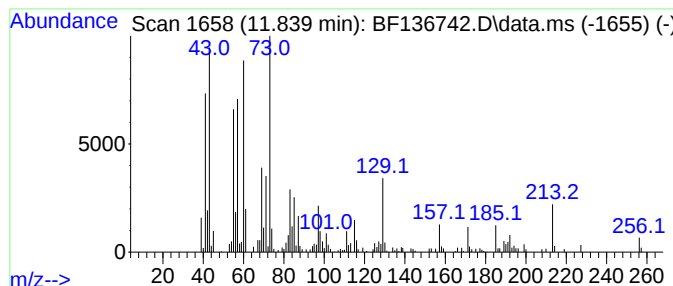
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	6.49 ng	138211	Phenanthrene-d10	11.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136742.D
Acq On : 27 Dec 2023 03:14
Operator : CG\JU
Sample : 05538-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-02-112223

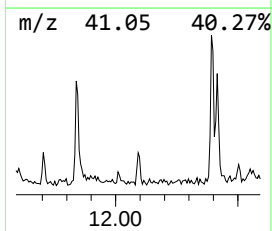
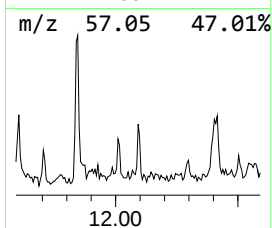
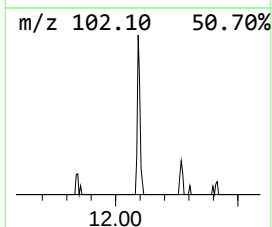
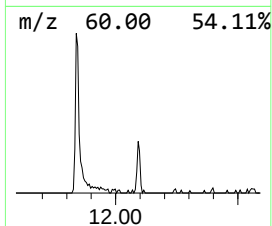
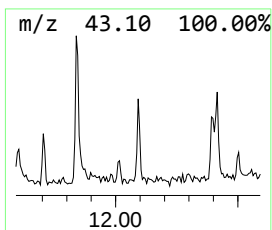
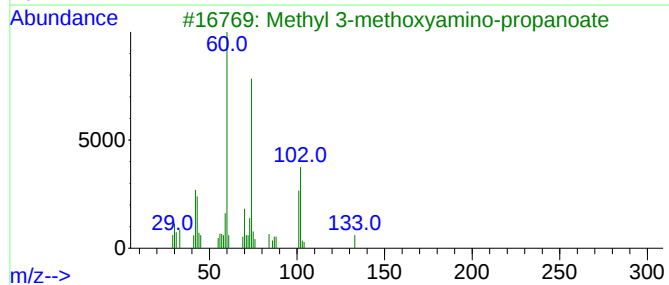
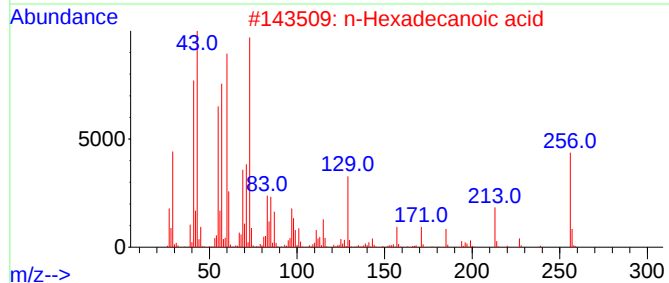
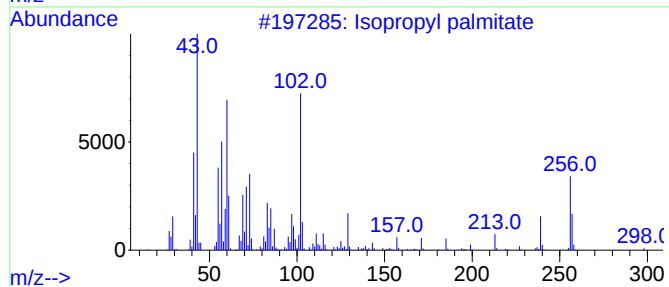
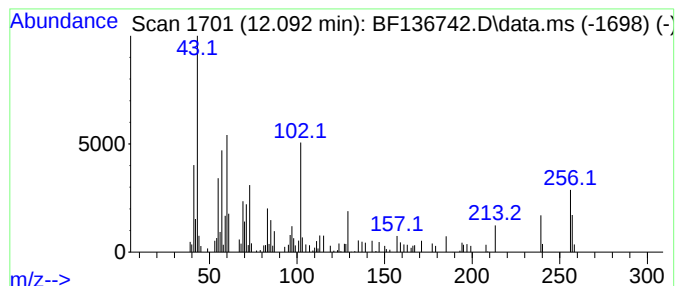
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Isopropyl palmitate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	2.28 ng	48508	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	80
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
3			Methyl 3-methoxyamino-propanoate	133	C5H11NO3	078191-05-6	38
4			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	25
5			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136742.D
Acq On : 27 Dec 2023 03:14
Operator : CG\JU
Sample : 05538-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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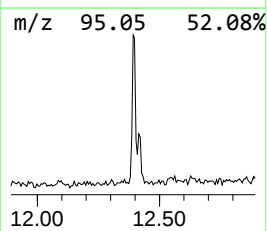
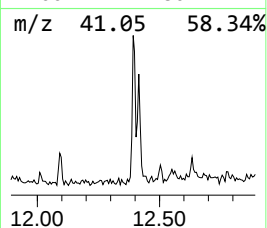
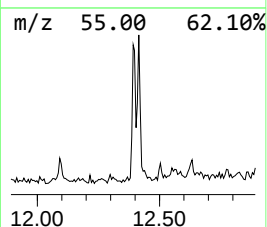
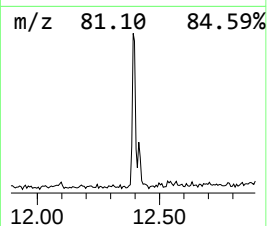
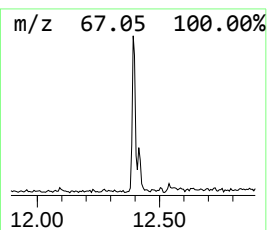
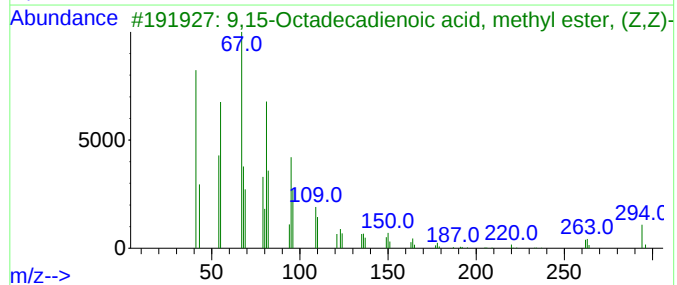
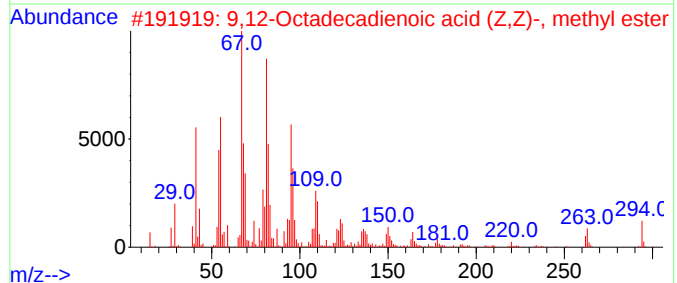
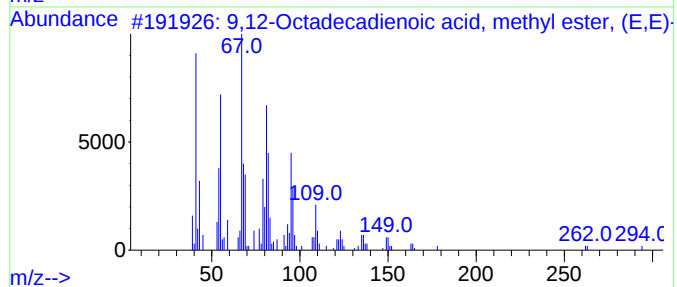
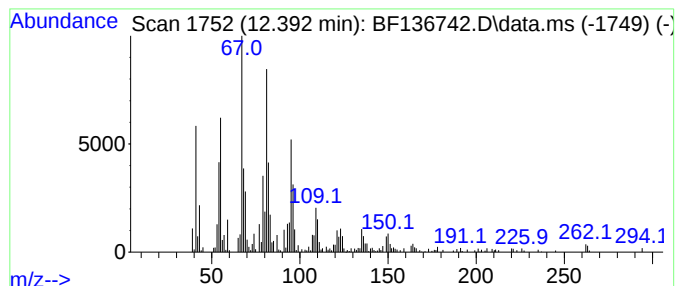
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.392	9.95 ng	211705	Phenanthrene-d10	11.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3		9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	97
4		9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	95
5		9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136742.D
Acq On : 27 Dec 2023 03:14
Operator : CG\JU
Sample : 05538-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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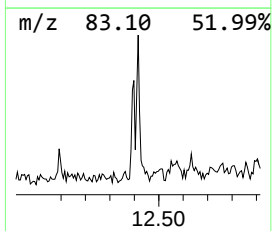
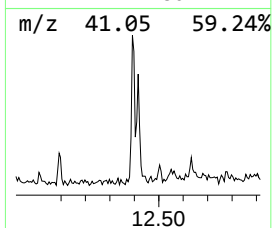
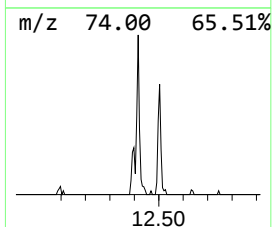
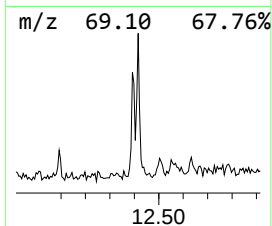
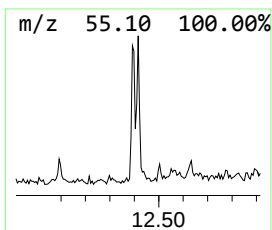
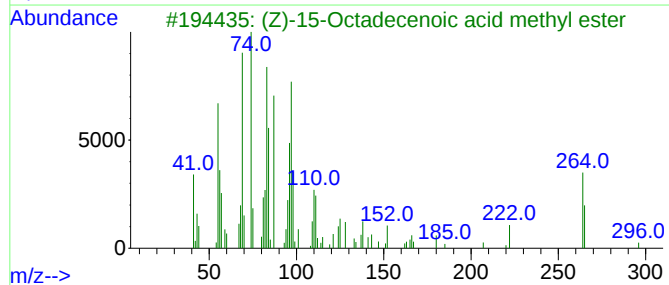
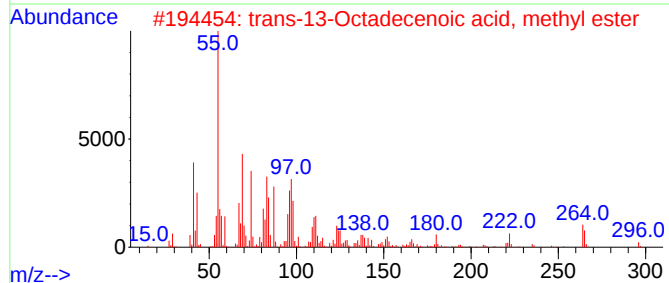
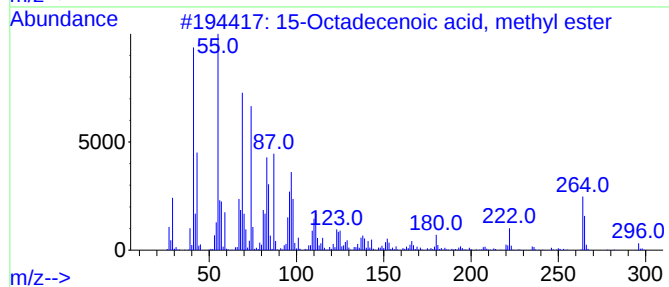
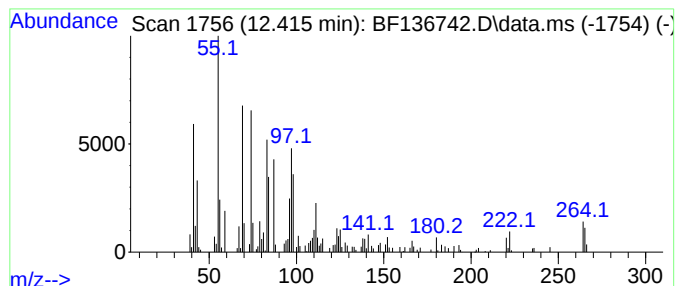
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 15-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	6.54 ng	139206	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	86
2			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	78
3			(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	78
4			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	78
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136742.D
Acq On : 27 Dec 2023 03:14
Operator : CG\JU
Sample : 05538-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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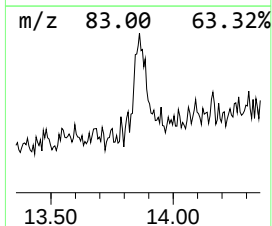
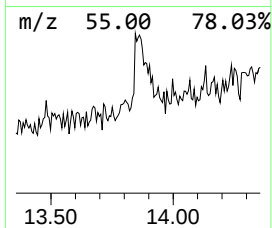
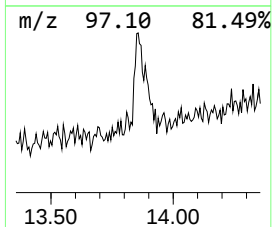
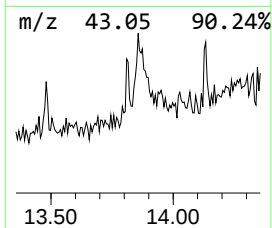
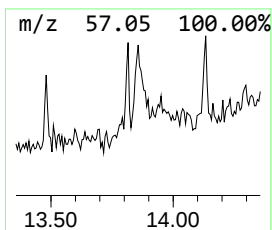
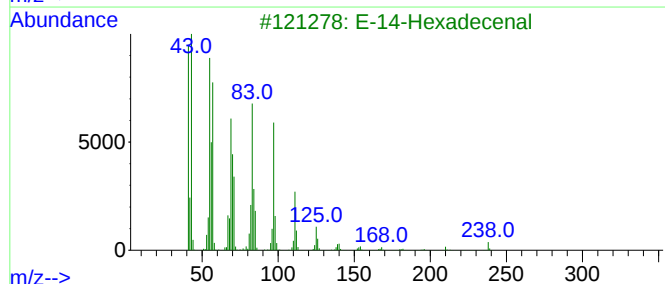
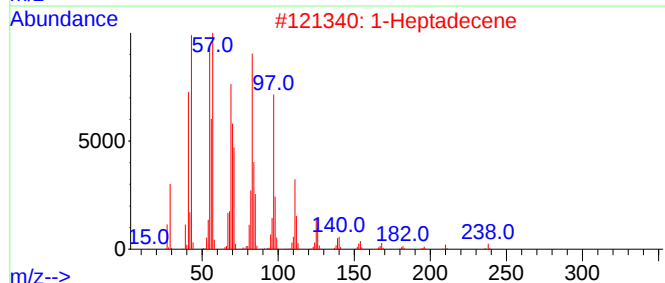
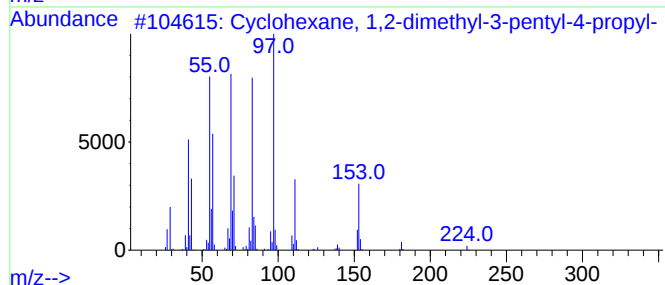
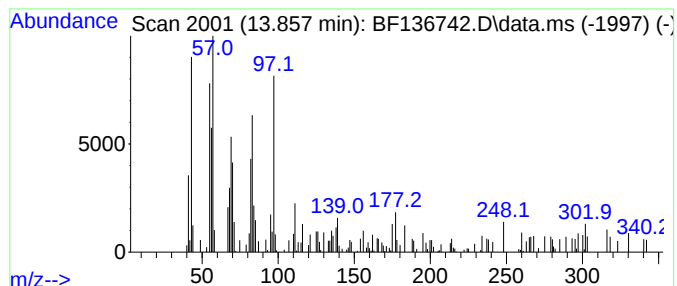
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.71 ng	54323	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	60
2			1-Heptadecene	238	C17H34	006765-39-5	51
3			E-14-Hexadecenal	238	C16H30O	330207-53-9	50
4			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	49
5			2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136742.D
Acq On : 27 Dec 2023 03:14
Operator : CG\JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
HR-02-112223

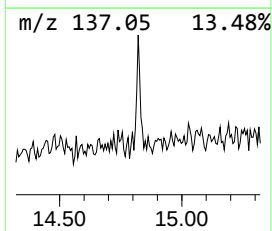
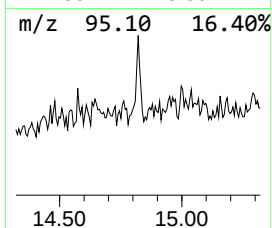
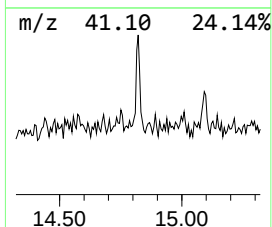
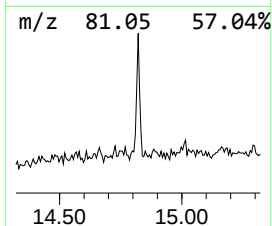
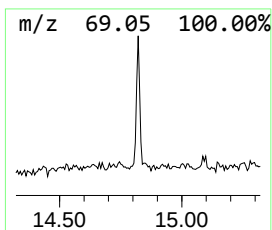
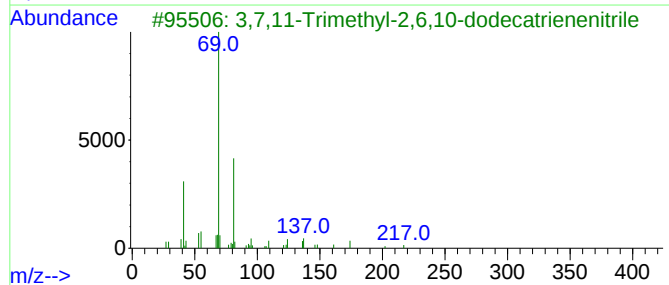
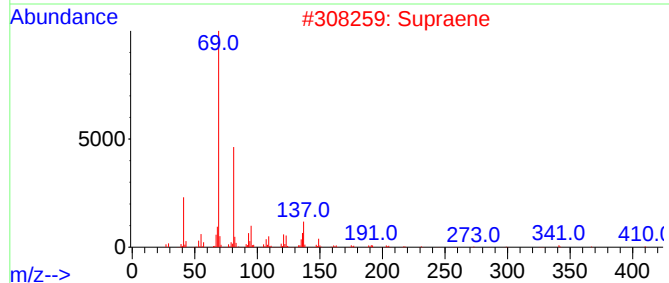
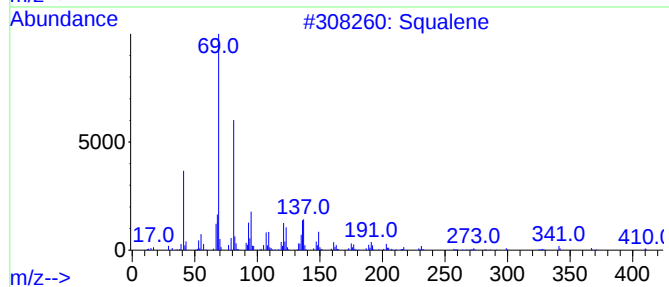
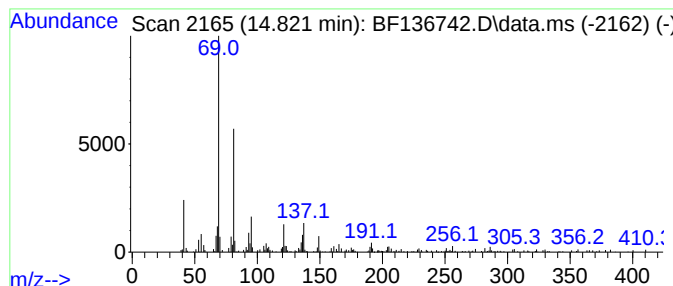
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	6.17 ng	72716	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	86
2			Supraene	410	C30H50	007683-64-9	72
3			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
4			1,2-Epoxy-3,7,11-trimethyl-(6E,1...	238	C15H26O2	1000432-46-2	59
5			6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122623\
Data File : BF136742.D
Acq On : 27 Dec 2023 03:14
Operator : CG\JU
Sample : 05538-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrame...	9.257	3.1	ng	67592	3	9.816	433866	20.0
3-Ethyl-2,6,10-...	9.539	2.0	ng	43549	3	9.816	433866	20.0
Tridecane, 5-pr...	10.733	2.7	ng	56843	4	11.310	425606	20.0
1-Octadecanesul...	11.604	2.1	ng	45500	4	11.310	425606	20.0
n-Hexadecanoic ...	11.839	6.5	ng	138211	4	11.310	425606	20.0
Isopropyl palmi...	12.092	2.3	ng	48508	4	11.310	425606	20.0
9,12-Octadecadi...	12.392	9.9	ng	211705	4	11.310	425606	20.0
15-Octadecenoic...	12.416	6.5	ng	139206	4	11.310	425606	20.0
Cyclohexane, 1,...	13.857	2.7	ng	54323	5	13.963	400468	20.0
Squalene	14.821	6.2	ng	72716	6	15.445	235583	20.0