

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010322\
 Data File : BF126464.D
 Acq On : 3 Jan 2022 19:30
 Operator : JU/CG
 Sample : M5253-01 2X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SA-1-122921

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126464.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	13	rVB	35202	47586	3.23%	0.307%
2	3.822	289	295	300	rVB	13733	20116	1.36%	0.130%
3	4.993	490	494	500	rVB	32088	35865	2.43%	0.232%
4	5.410	561	565	568	rBV	1603274	1475451	100.00%	9.531%
5	6.428	734	738	754	rBV	1575162	1406324	95.31%	9.085%
6	6.798	797	801	804	rBV	842611	666437	45.17%	4.305%
7	7.069	844	847	851	rVB2	13948	15855	1.07%	0.102%
8	7.357	892	896	899	rBV	1026295	834646	56.57%	5.392%
9	7.439	907	910	915	rBV6	12955	19388	1.31%	0.125%
10	7.969	994	1000	1002	rBV4	17843	23223	1.57%	0.150%
11	8.081	1015	1019	1026	rBV	995002	821984	55.71%	5.310%
12	8.257	1042	1049	1052	rBV7	13075	27633	1.87%	0.179%
13	8.292	1052	1055	1057	rVB	29985	25240	1.71%	0.163%
14	8.375	1065	1069	1072	rBV4	15768	24660	1.67%	0.159%
15	8.510	1089	1092	1094	rBV	33925	33327	2.26%	0.215%
16	8.628	1108	1112	1114	rBV3	22586	24036	1.63%	0.155%
17	8.681	1117	1121	1123	rBV2	20886	24638	1.67%	0.159%
18	8.963	1166	1169	1172	rBV3	14484	18006	1.22%	0.116%
19	9.110	1191	1194	1198	rVB2	47167	46910	3.18%	0.303%
20	9.157	1198	1202	1205	rBV	1587325	1286653	87.20%	8.312%
21	9.245	1214	1217	1221	rVB	52606	49498	3.35%	0.320%
22	9.298	1221	1226	1227	rBV5	13534	19928	1.35%	0.129%
23	9.563	1266	1271	1273	rBV2	39470	50891	3.45%	0.329%
24	9.645	1283	1285	1292	rVB8	12775	19181	1.30%	0.124%
25	9.769	1304	1306	1309	rVB	35641	28649	1.94%	0.185%
26	9.833	1311	1317	1321	rBV	1025692	866961	58.76%	5.601%
27	10.245	1385	1387	1389	rBV2	24911	25061	1.70%	0.162%
28	10.269	1389	1391	1395	rVV	42551	37282	2.53%	0.241%
29	10.327	1399	1401	1407	rVB6	10830	17419	1.18%	0.113%
30	10.492	1426	1429	1434	rVB	25411	25136	1.70%	0.162%
31	10.622	1447	1451	1455	rBV	890416	773163	52.40%	4.995%
32	10.745	1469	1472	1480	rVB	53519	75807	5.14%	0.490%
33	11.192	1546	1548	1550	rBV2	41591	32014	2.17%	0.207%
34	11.222	1550	1553	1560	rVB2	33251	38781	2.63%	0.251%
35	11.280	1560	1563	1566	rBV5	18478	19438	1.32%	0.126%
36	11.322	1566	1570	1572	rBV	969112	862961	58.49%	5.575%

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37	11.345	1572	1574	1576	rVB	59803	45274	3.07%	0.292%
38	11.616	1618	1620	1623	rBV	32725	31607	2.14%	0.204%
39	11.716	1634	1637	1641	rBV	435683	375840	25.47%	2.428%
40	11.786	1645	1649	1652	rBV5	14315	21373	1.45%	0.138%
41	11.822	1652	1655	1657	rBV	19430	18268	1.24%	0.118%
42	11.851	1657	1660	1664	rBV2	84012	100480	6.81%	0.649%
43	12.027	1687	1690	1693	rVB	35738	25889	1.75%	0.167%
44	12.304	1734	1737	1742	rVB7	19058	31193	2.11%	0.202%
45	12.404	1751	1754	1756	rBV	1125278	1012538	68.63%	6.541%
46	12.427	1756	1758	1760	rVB	1033811	804667	54.54%	5.198%
47	12.510	1769	1772	1774	rBV	241689	196564	13.32%	1.270%
48	12.527	1774	1775	1779	rVB	80926	68783	4.66%	0.444%
49	12.639	1792	1794	1798	rBV5	18083	19438	1.32%	0.126%
50	12.757	1810	1814	1817	rBV	94850	104737	7.10%	0.677%
51	12.786	1817	1819	1822	rVB	33951	28682	1.94%	0.185%
52	12.904	1835	1839	1843	rBV	1479379	1282649	86.93%	8.286%
53	13.145	1877	1880	1885	rVB2	37111	57248	3.88%	0.370%
54	13.233	1893	1895	1898	rBV3	28756	28468	1.93%	0.184%
55	13.451	1929	1932	1935	rBV	88624	83200	5.64%	0.537%
56	13.486	1936	1938	1940	rVV	39979	30853	2.09%	0.199%
57	13.815	1990	1994	2001	rVB3	133902	191366	12.97%	1.236%
58	13.957	2014	2018	2021	rBV	701368	656946	44.53%	4.244%
59	15.404	2260	2264	2267	rBV	366710	443700	30.07%	2.866%

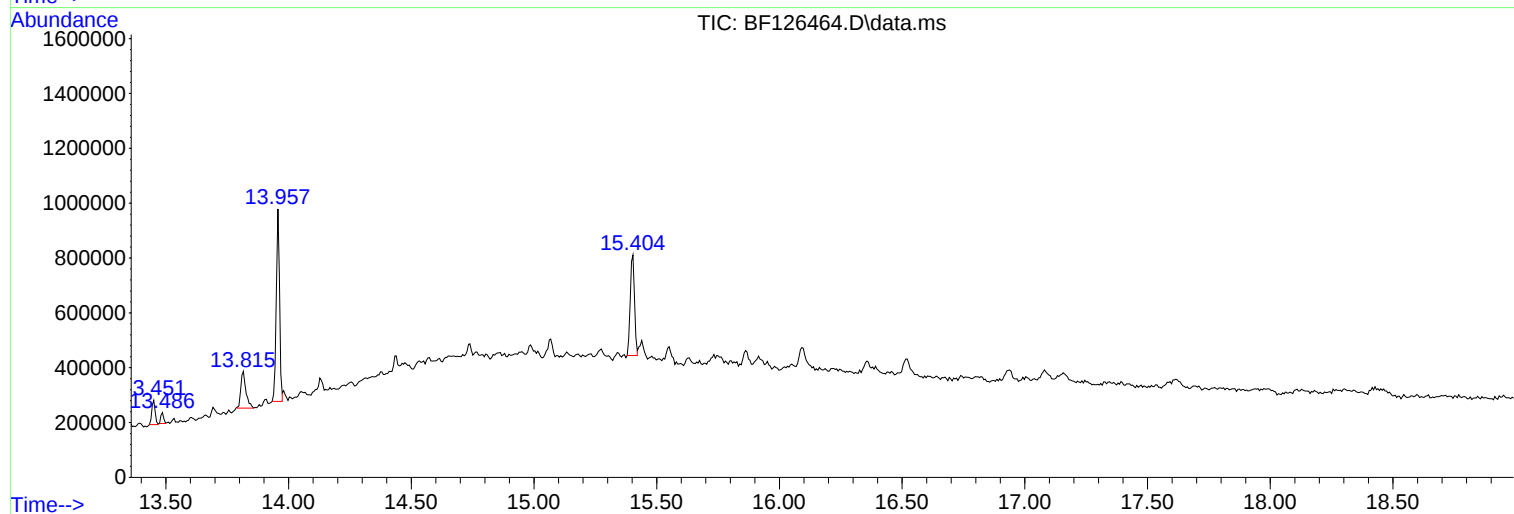
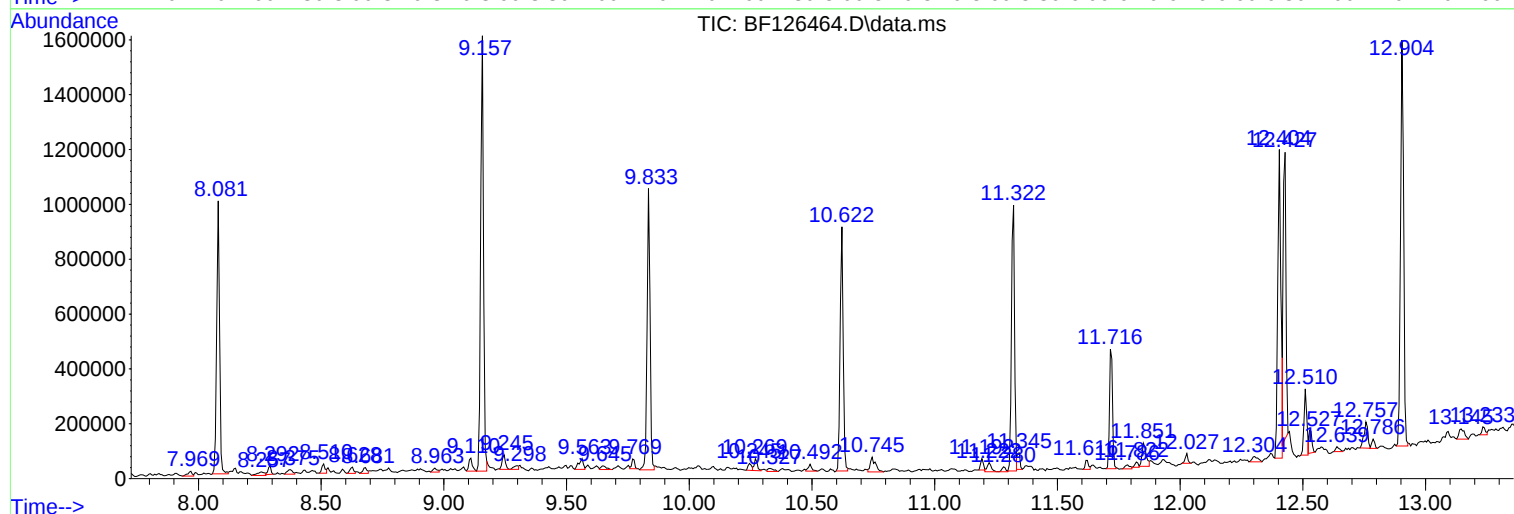
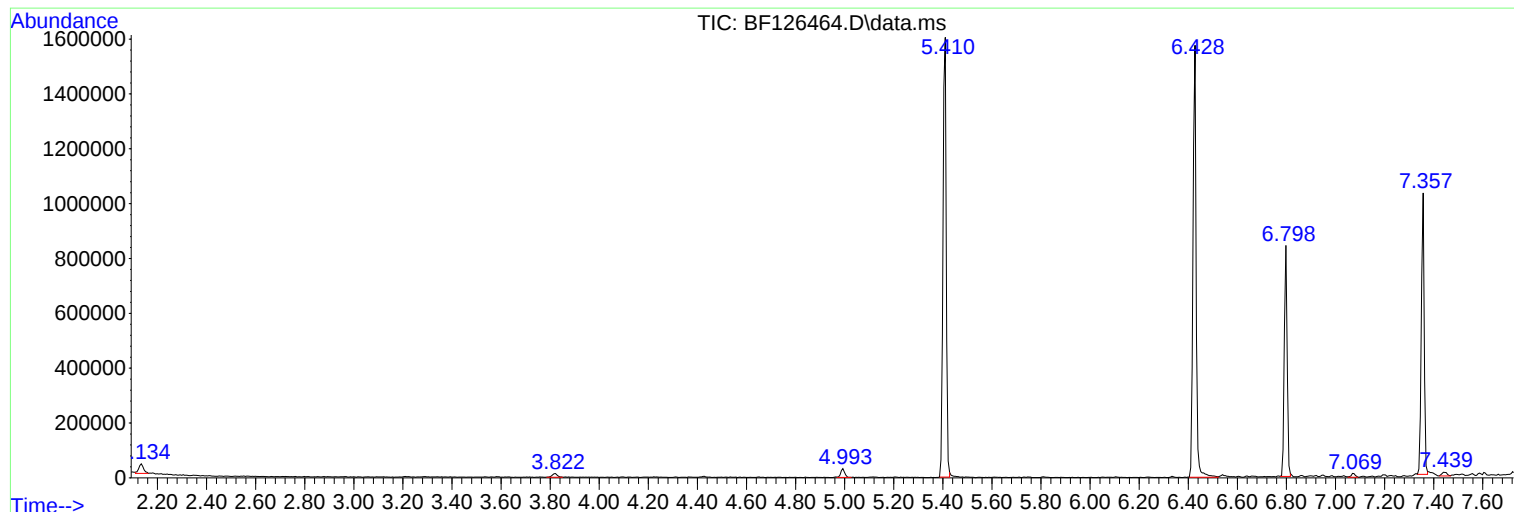
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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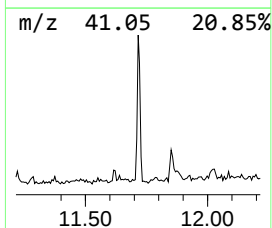
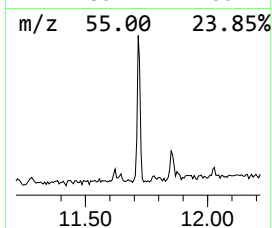
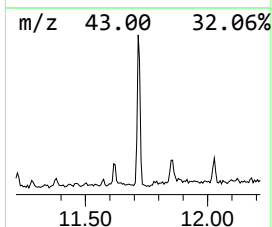
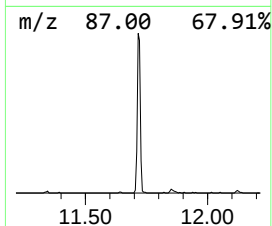
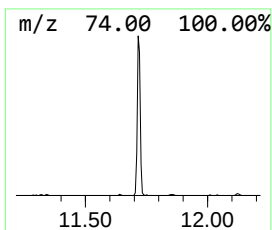
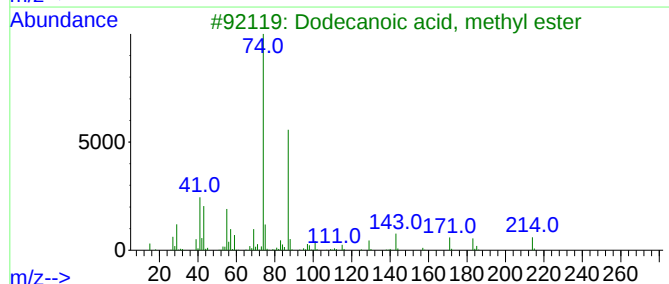
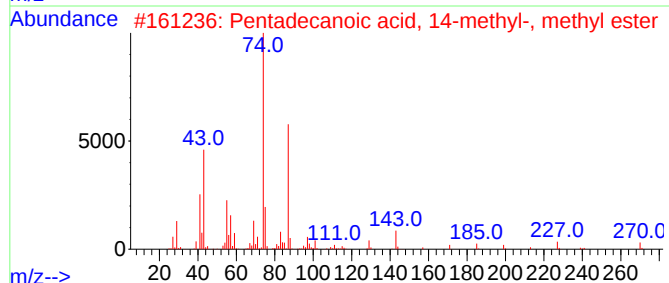
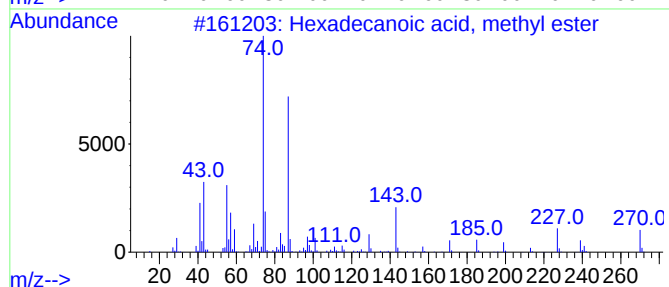
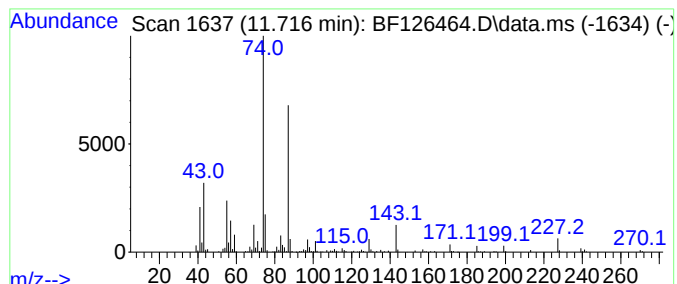
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.716	8.71 ng	375840	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	91
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
5			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	90



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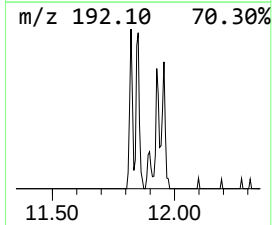
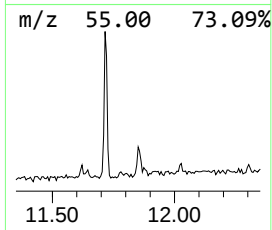
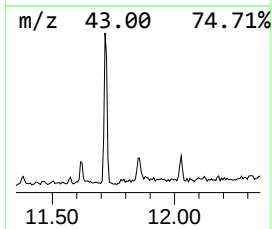
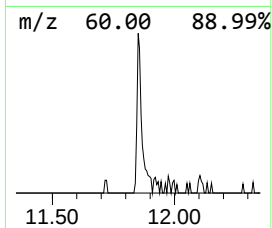
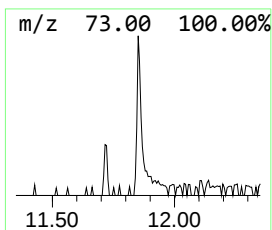
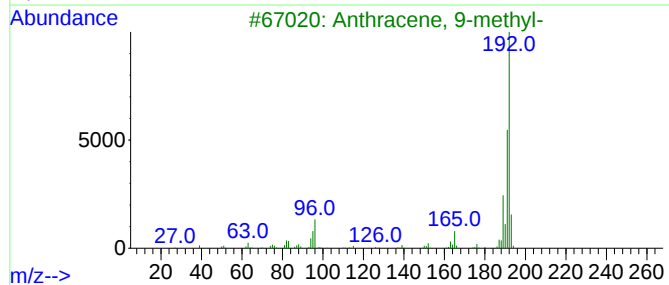
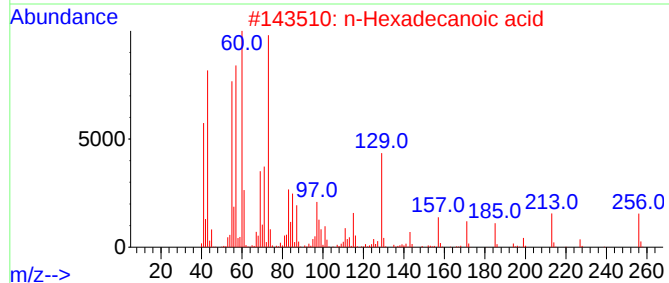
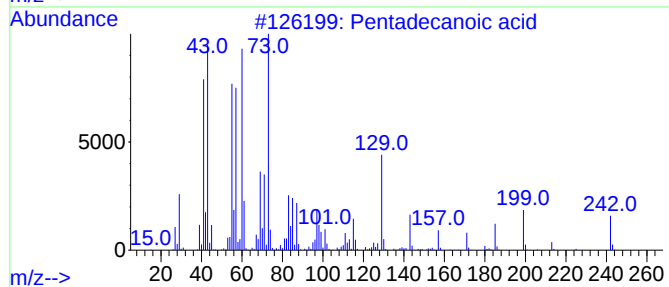
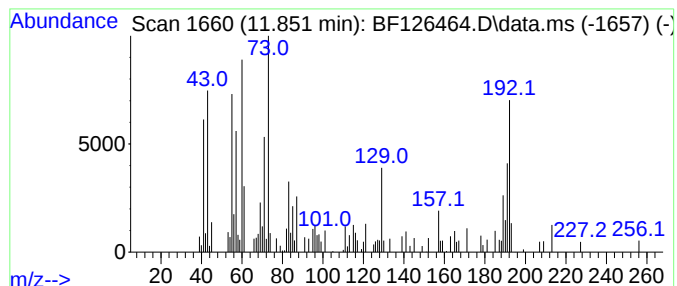
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown11.851 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.851	2.33 ng	100480	Phenanthrene-d10	11.322	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	25
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	25
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	18



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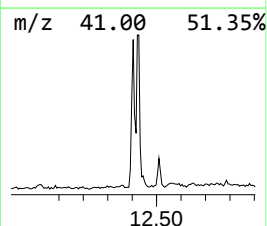
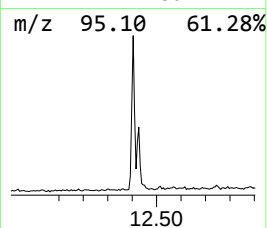
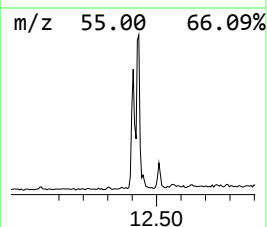
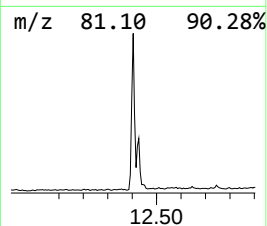
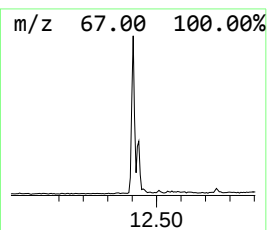
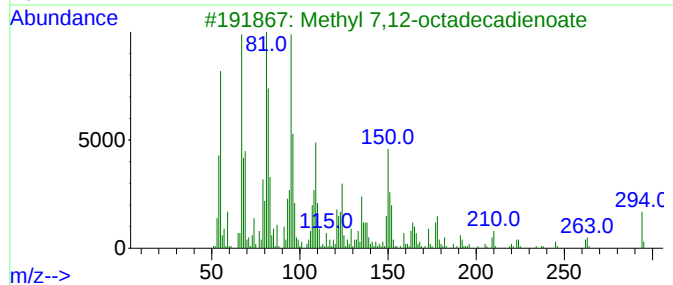
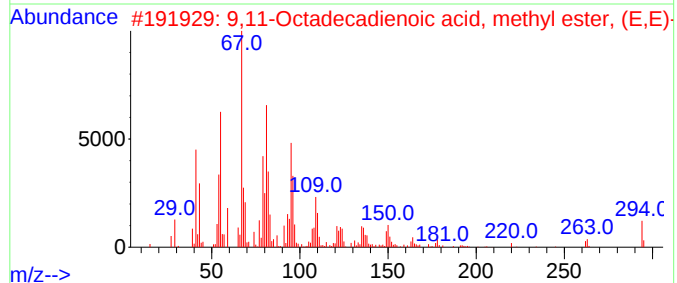
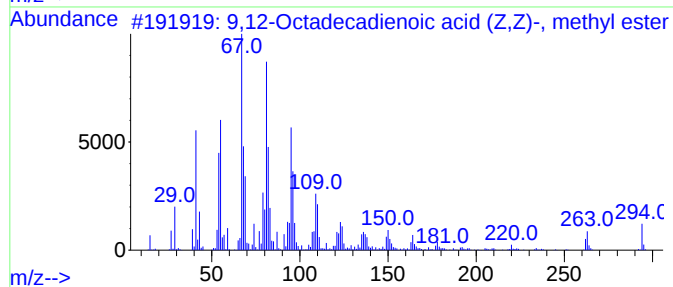
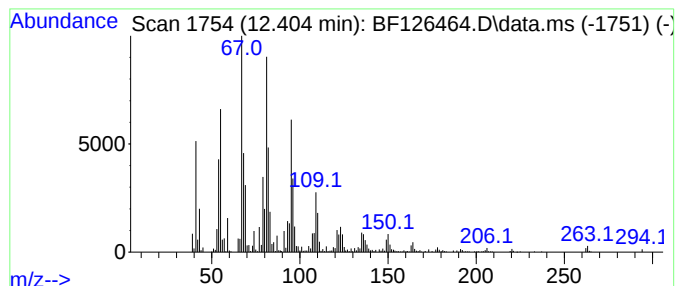
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.404	23.47 ng	1012540	Phenanthrene-d10	11.322	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	96
3	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	95
4	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
5	Linolaidic acid	280	C18H32O2	000506-21-8	95



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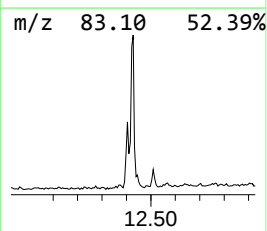
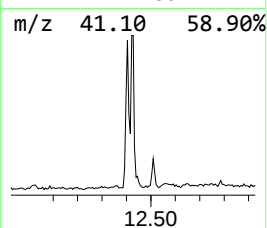
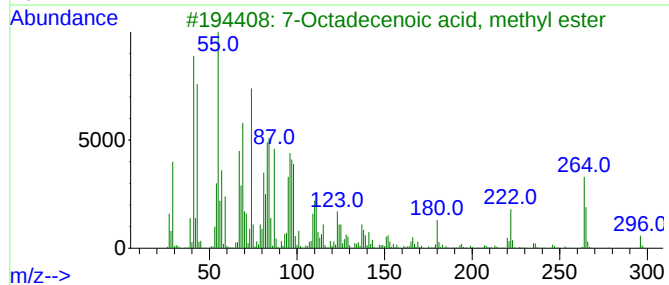
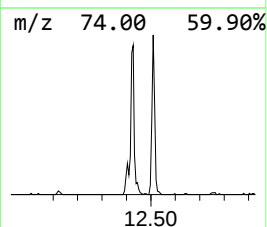
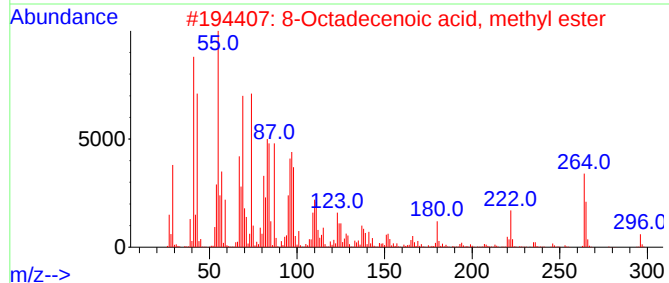
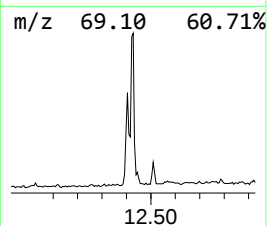
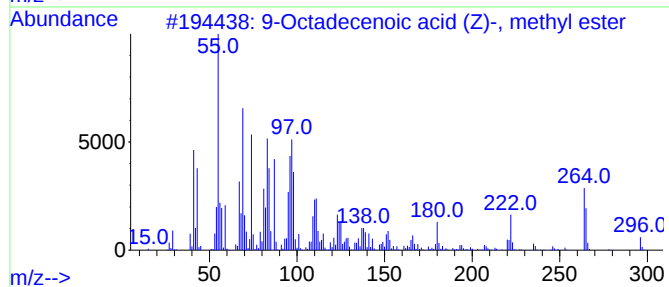
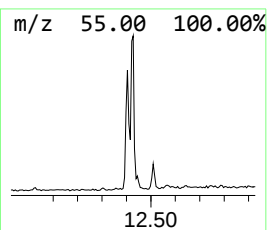
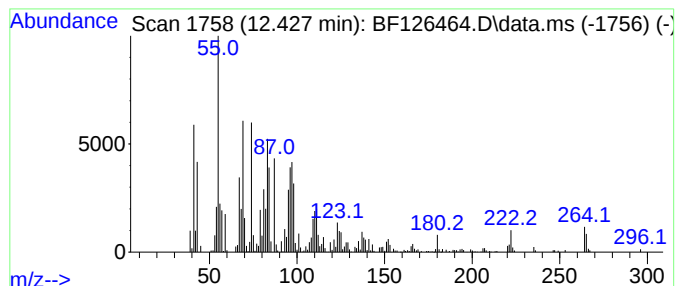
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	18.65 ng	804667	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99		
2	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99		
3	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99		
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99		
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99		



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ClientSampleId :
SA-1-122921

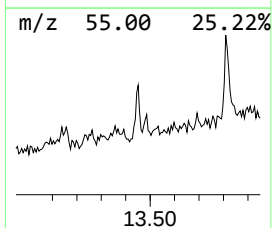
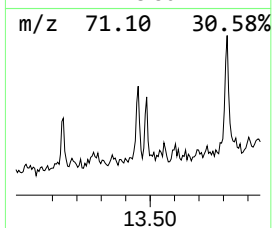
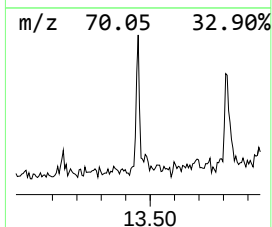
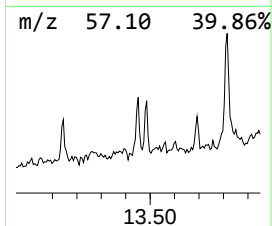
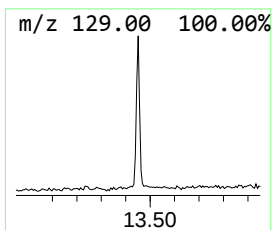
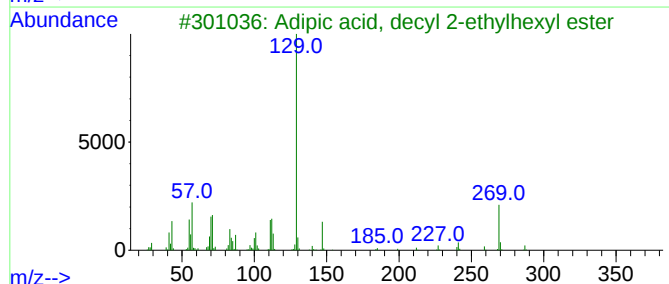
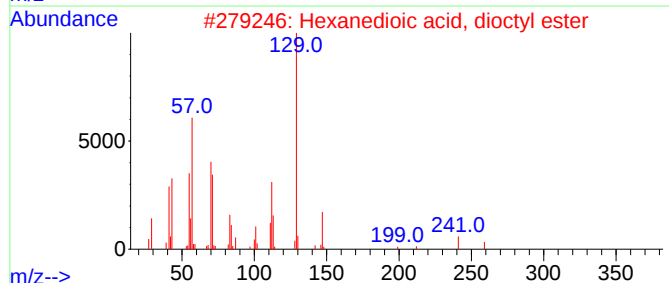
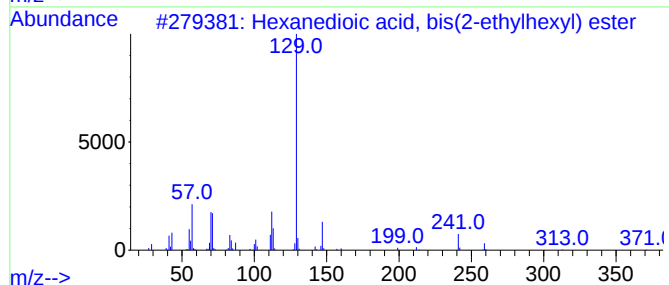
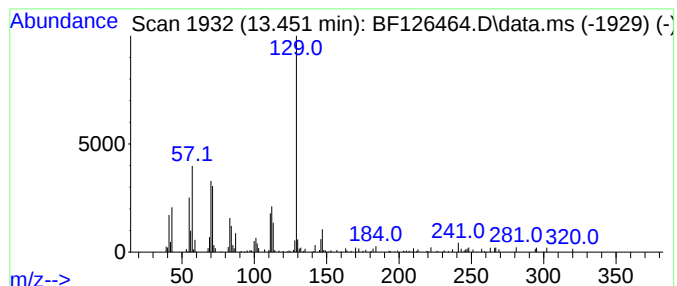
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.451	2.53 ng	83200	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	62
3			Adipic acid, decyl 2-ethylhexyl ...	398	C24H46O4	1000324-48-8	59
4			Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	49
5			Adipic acid, octyl trans-2-methy...	354	C21H38O4	1000324-75-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010322\
Data File : BF126464.D
Acq On : 3 Jan 2022 19:30
Operator : JU/CG
Sample : M5253-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-1-122921

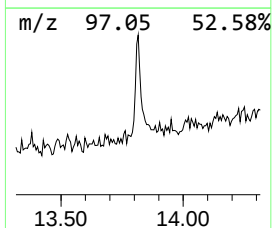
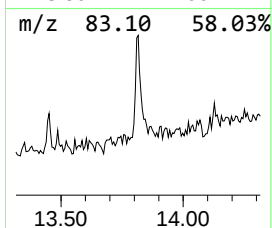
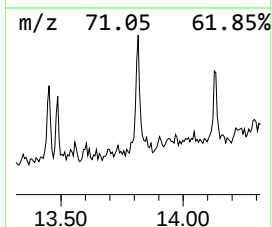
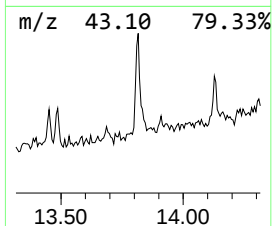
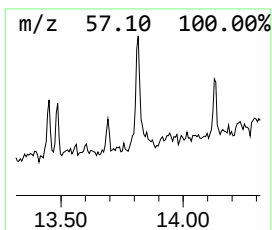
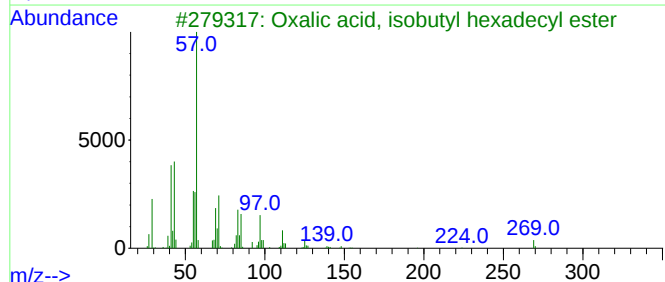
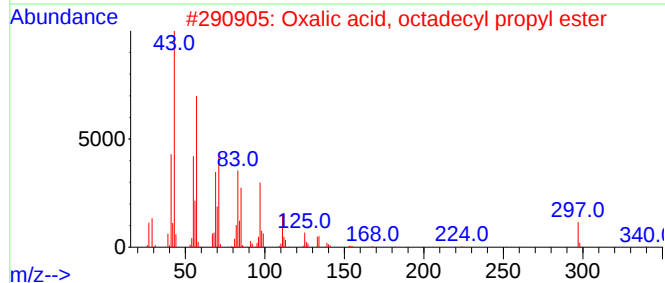
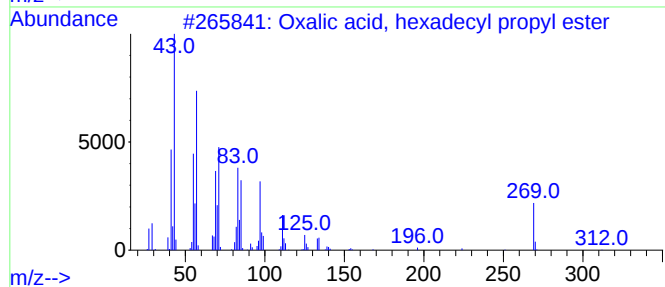
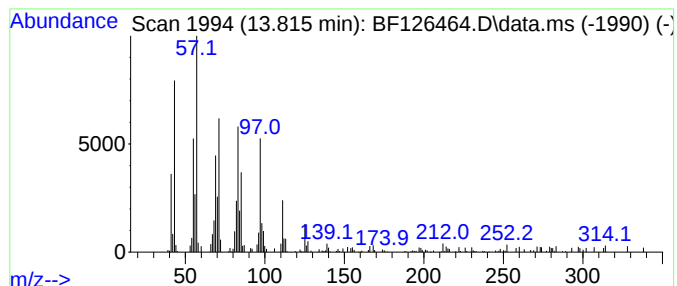
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Oxalic acid, hexadecyl prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	5.83 ng	191366	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
2			Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	91
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010322\
Data File : BF126464.D
Acq On : 3 Jan 2022 19:30
Operator : JU/CG
Sample : M5253-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-1-122921

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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
Hexadecanoic ac...	11.716	8.7	ng	375840	4	11.322	862961	20.0
unknown11.851	11.851	2.3	ng	100480	4	11.322	862961	20.0
9,12-Octadecadi...	12.404	23.5	ng	1012540	4	11.322	862961	20.0
9-Octadecenoic ...	12.427	18.6	ng	804667	4	11.322	862961	20.0
Hexanedioic aci...	13.451	2.5	ng	83200	5	13.957	656946	20.0
Oxalic acid, he...	13.816	5.8	ng	191366	5	13.957	656946	20.0