

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
 Data File : BF123832.D
 Acq On : 5 May 2021 17:36
 Operator : JU/CG
 Sample : M2279-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EME-14

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-BF042721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123832.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	490	493	503	rVB	70165	97904	1.96%	0.237%
2	5.410	561	565	577	rBV	5255385	4760669	95.10%	11.526%
3	6.434	735	739	742	rBV	5613296	5005735	100.00%	12.119%
4	6.792	796	800	803	rBV	1811443	1365112	27.27%	3.305%
5	7.357	891	896	899	rBV	3869506	3200208	63.93%	7.748%
6	8.075	1013	1018	1022	rBV	2097783	1850913	36.98%	4.481%
7	9.157	1198	1202	1205	rBV	6295161	4811801	96.13%	11.649%
8	9.239	1212	1216	1219	rBV	78617	70083	1.40%	0.170%
9	9.422	1243	1247	1250	rBV4	44951	61010	1.22%	0.148%
10	9.492	1254	1259	1261	rBV	81403	76625	1.53%	0.186%
11	9.551	1266	1269	1272	rBV	287774	264704	5.29%	0.641%
12	9.833	1313	1317	1320	rBV	2537253	1945983	38.88%	4.711%
13	9.863	1320	1322	1326	rVB	98245	84649	1.69%	0.205%
14	10.380	1407	1410	1414	rBV	116356	98668	1.97%	0.239%
15	10.621	1447	1451	1455	rBV	3835206	3283246	65.59%	7.949%
16	10.745	1469	1472	1476	rBV3	112949	154757	3.09%	0.375%
17	10.810	1479	1483	1485	rBV	103953	104437	2.09%	0.253%
18	10.839	1485	1488	1492	rVB2	102132	115607	2.31%	0.280%
19	10.874	1492	1494	1496	rBV	89209	75401	1.51%	0.183%
20	11.069	1524	1527	1531	rVB4	61334	69130	1.38%	0.167%
21	11.192	1542	1548	1550	rBV4	61392	75923	1.52%	0.184%
22	11.216	1550	1552	1557	rVB2	68710	77424	1.55%	0.187%
23	11.321	1566	1570	1572	rBV	2342777	1846282	36.88%	4.470%
24	11.345	1572	1574	1577	rVV	488989	369222	7.38%	0.894%
25	11.392	1577	1582	1585	rVB2	170673	207530	4.15%	0.502%
26	11.821	1652	1655	1658	rBV	129456	117509	2.35%	0.284%
27	11.857	1658	1661	1664	rBV2	264022	266731	5.33%	0.646%
28	11.933	1671	1674	1676	rBV2	166650	173743	3.47%	0.421%
29	11.957	1676	1678	1682	rVB	98992	83190	1.66%	0.201%
30	12.374	1746	1749	1751	rBV	83513	86590	1.73%	0.210%
31	12.404	1751	1754	1760	rVB5	183418	263277	5.26%	0.637%
32	12.533	1773	1776	1780	rBV	411635	336830	6.73%	0.815%
33	12.763	1810	1815	1818	rBV	470262	450077	8.99%	1.090%
34	12.792	1818	1820	1828	rVB4	96449	160330	3.20%	0.388%
35	12.910	1836	1840	1843	rBV	4131431	3449089	68.90%	8.350%
36	13.092	1869	1871	1874	rVB	87182	81457	1.63%	0.197%

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Min Area: 3 % of largest Peak

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

Peak separation: 5

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37	13.151	1877	1881	1885	rVV2	80703	132321	2.64%	0.320%
38	13.198	1886	1889	1892	rVV	68789	67121	1.34%	0.162%
39	13.321	1907	1910	1913	rBV2	70812	68106	1.36%	0.165%
40	13.492	1936	1939	1942	rBV	81208	78861	1.58%	0.191%
41	13.821	1992	1995	2007	rVB3	324702	598168	11.95%	1.448%
42	13.962	2015	2019	2022	rBV2	1342920	1402474	28.02%	3.395%
43	13.992	2022	2024	2027	rVB	163433	126461	2.53%	0.306%
44	14.139	2046	2049	2051	rVB	110850	97843	1.95%	0.237%
45	14.445	2098	2101	2104	rBV	179342	180393	3.60%	0.437%
46	14.745	2149	2152	2155	rBV	145200	139221	2.78%	0.337%
47	14.821	2162	2165	2172	rVB	148348	150099	3.00%	0.363%
48	14.998	2192	2195	2198	rBV2	137737	187213	3.74%	0.453%
49	15.080	2206	2209	2213	rBV	177631	168851	3.37%	0.409%
50	15.298	2243	2246	2251	rVB	85990	101828	2.03%	0.247%
51	15.356	2253	2256	2262	rVB	126046	157346	3.14%	0.381%
52	15.421	2262	2267	2271	rBV	1016626	1221634	24.40%	2.958%
53	15.886	2342	2346	2352	rVB	151435	198571	3.97%	0.481%
54	16.315	2415	2419	2421	rBV5	54689	88564	1.77%	0.214%
55	17.474	2610	2616	2628	rVB8	204441	598606	11.96%	1.449%

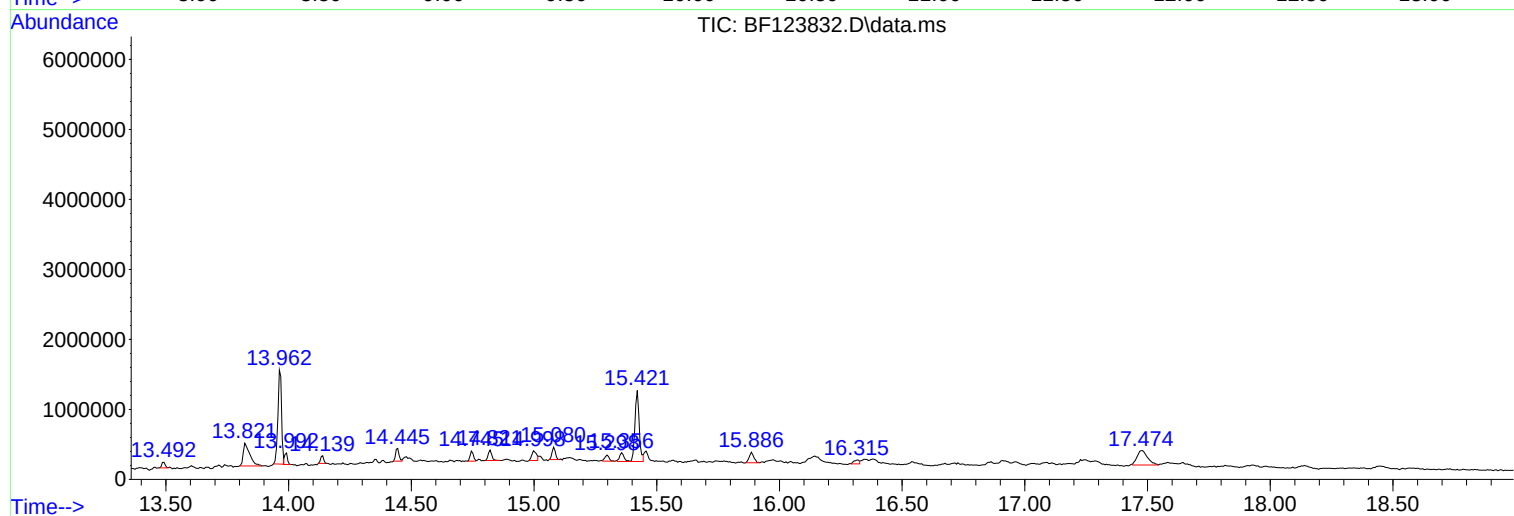
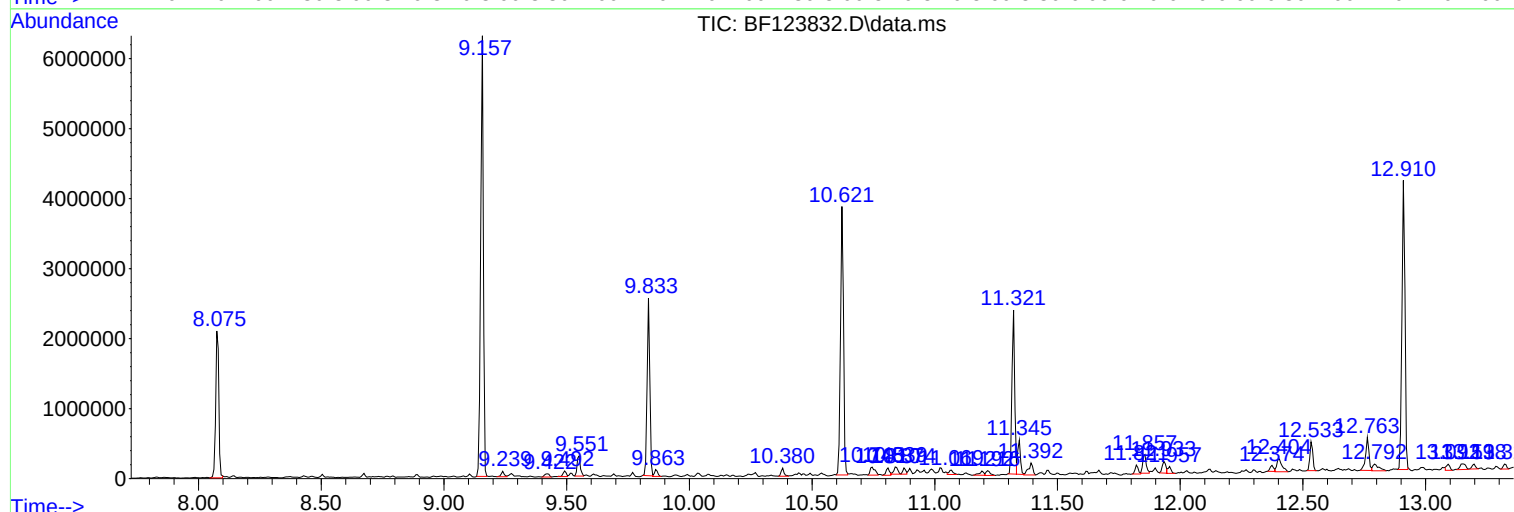
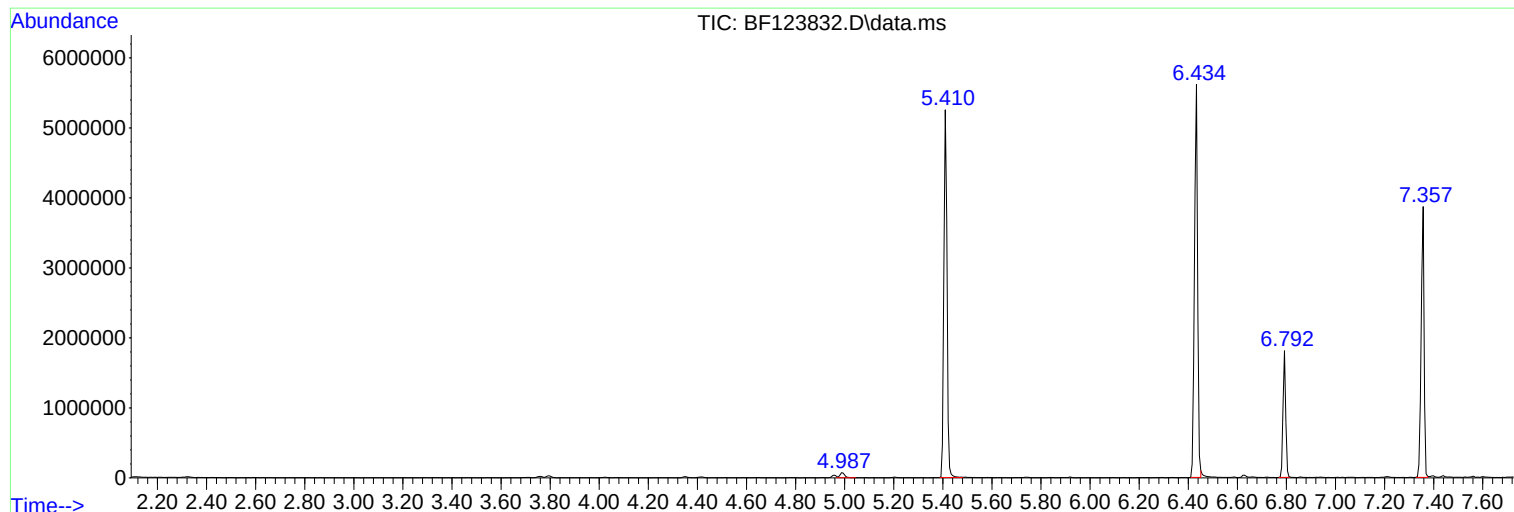
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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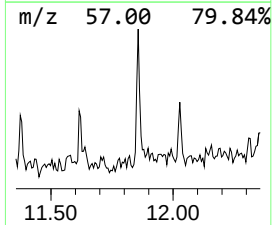
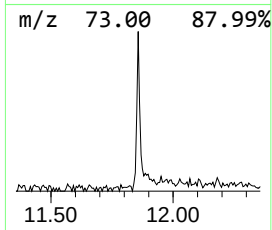
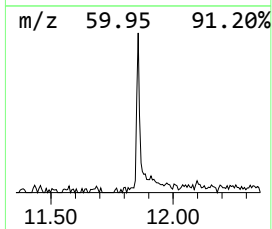
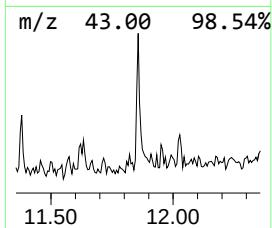
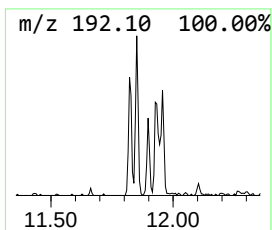
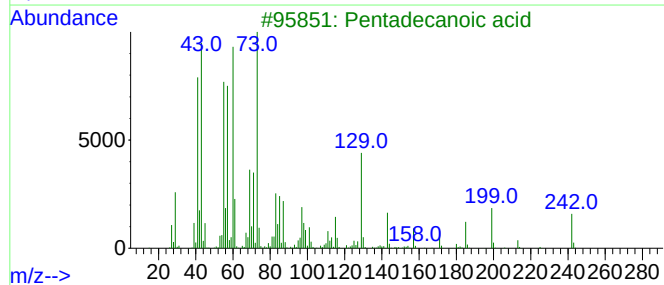
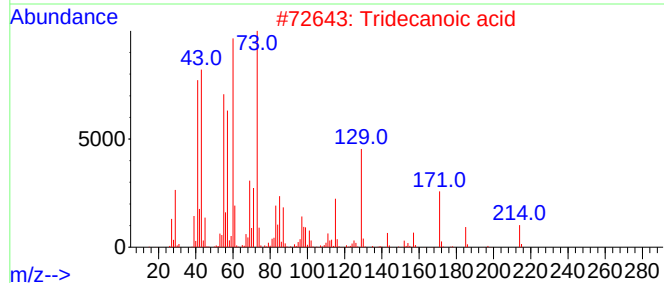
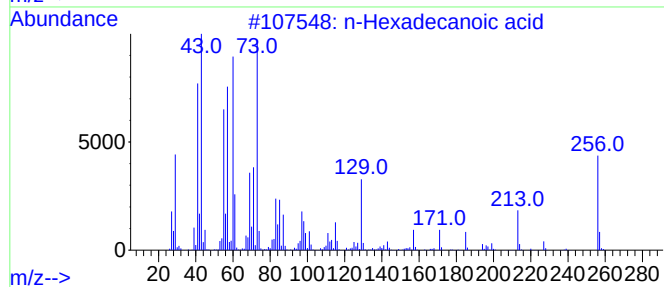
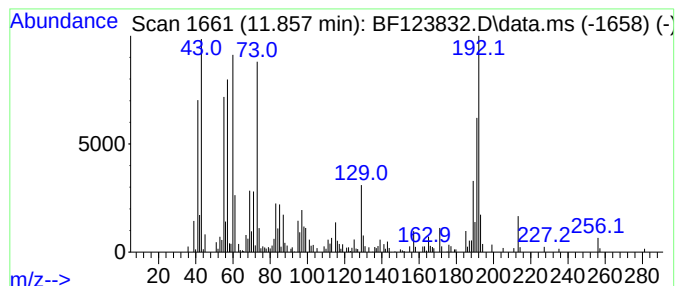
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	2.89 ng	266731	Phenanthrene-d10	11.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4			n-Decanoic acid	172	C10H20O2	000334-48-5	42
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38



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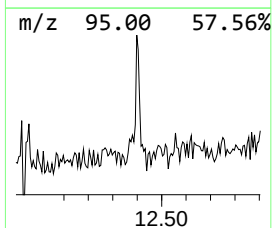
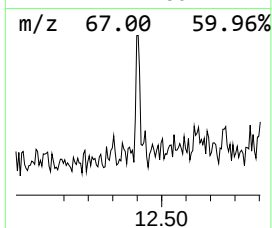
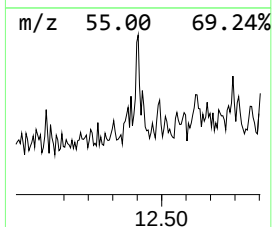
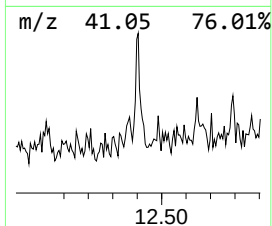
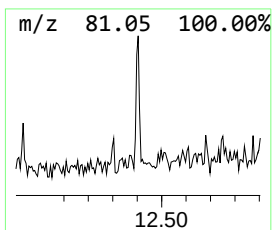
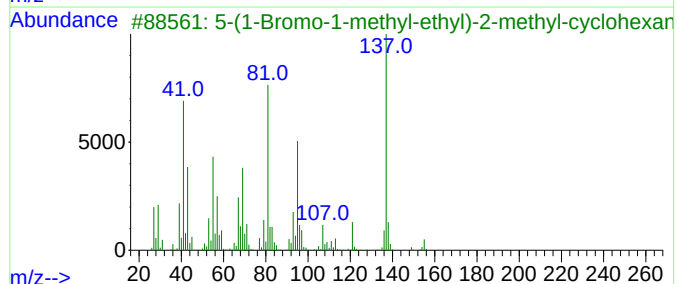
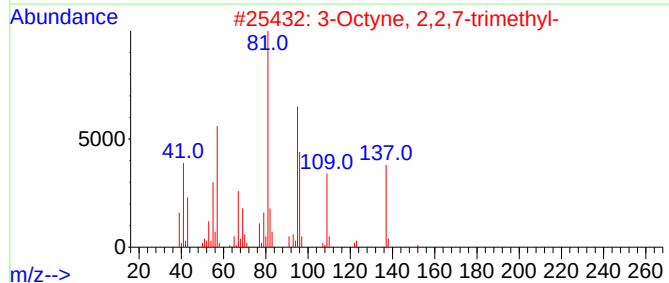
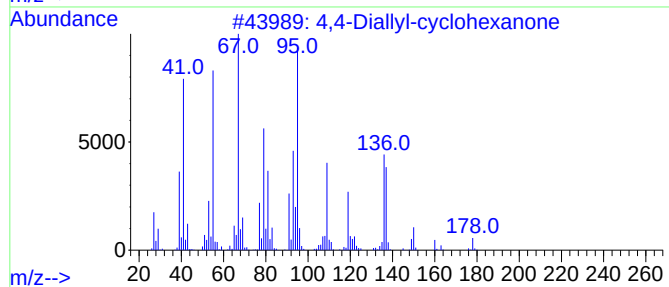
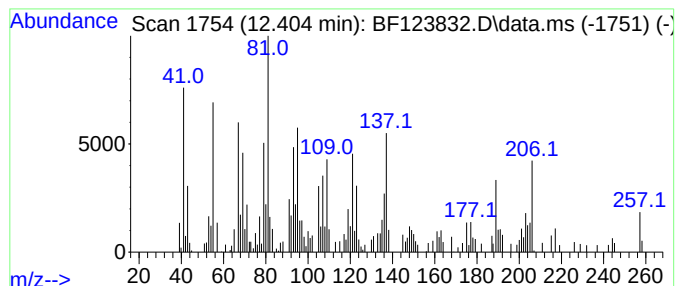
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 4,4-Diallyl-cyclohexanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.404	2.85 ng	263277	Phenanthrene-d10	11.321

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4-Diallyl-cyclohexanone	178	C12H18O	1000186-50-2	74
2			3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	43
3			5-(1-Bromo-1-methyl-ethyl)-2-met...	234	C10H19BrO	1000188-65-7	38
4			2(1H)-Pyridinone, 1-ethyl-6-methyl-	137	C8H11NO	019038-36-9	25
5			2(1H)-Pyridone, 1-ethyl-4-methyl-	137	C8H11NO	019006-62-3	25



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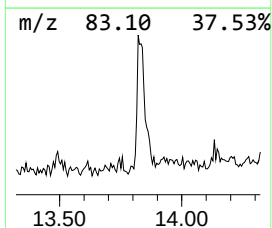
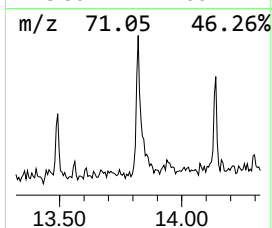
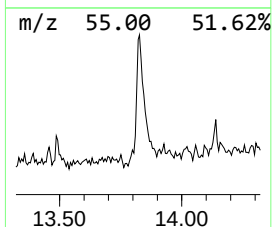
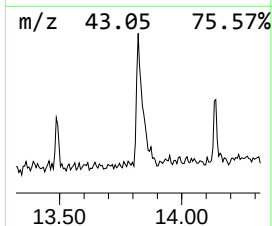
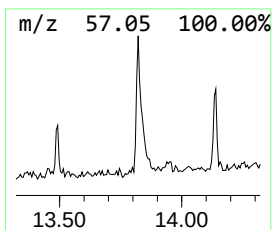
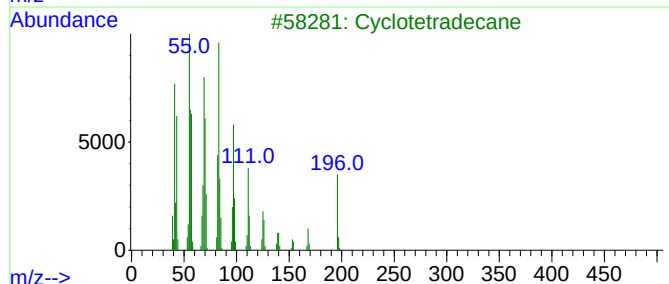
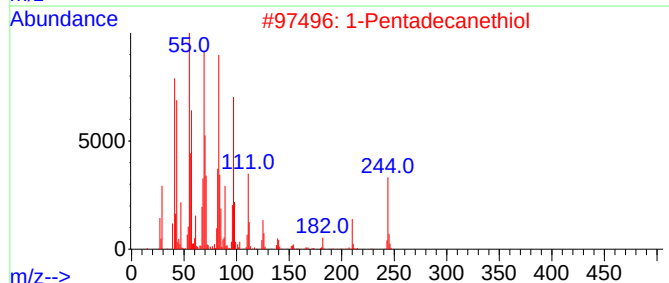
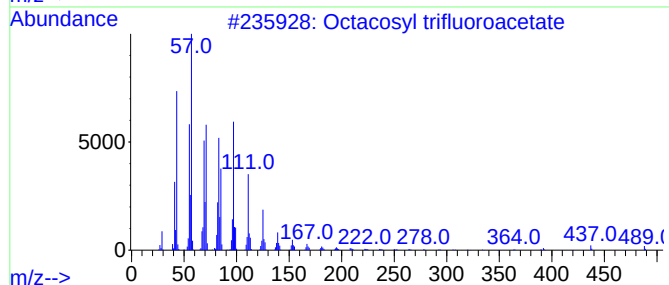
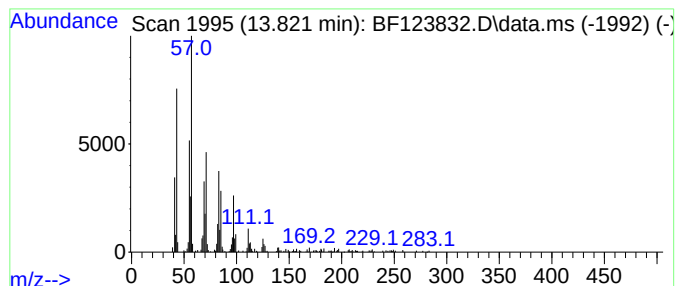
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octacosyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	8.53 ng	598168	Chrysene-d12	13.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
2			1-Pentadecanethiol	244	C15H32S	025276-70-4	87
3			Cyclotetradecane	196	C14H28	000295-17-0	86
4			Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	86
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	86



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Instrument :
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ClientSampled :
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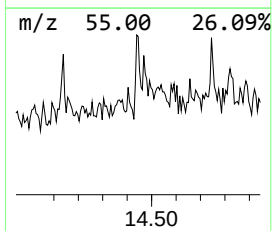
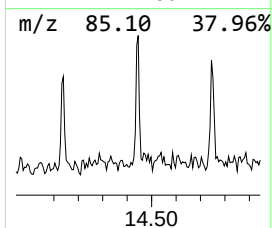
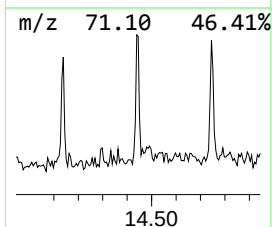
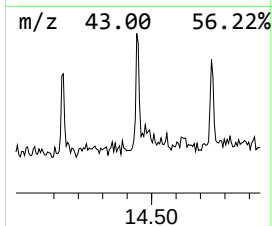
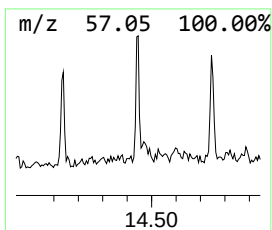
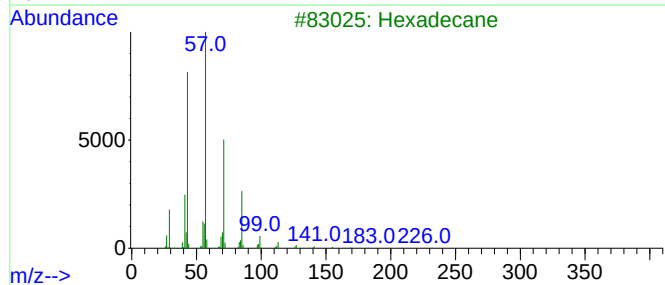
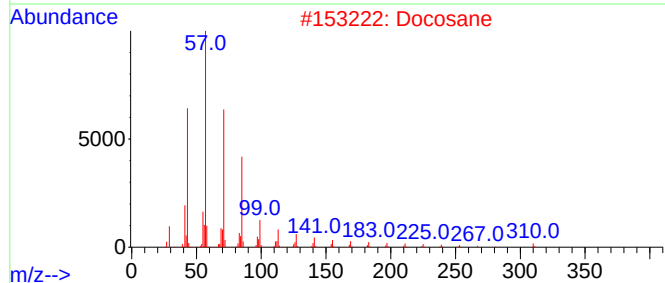
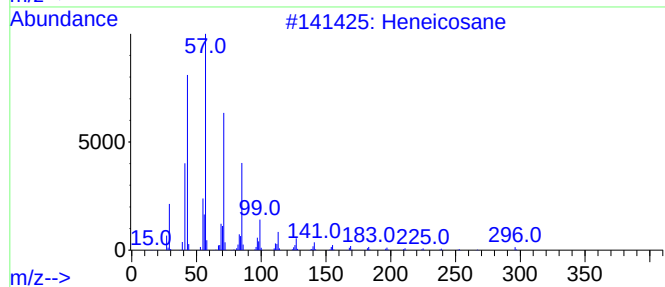
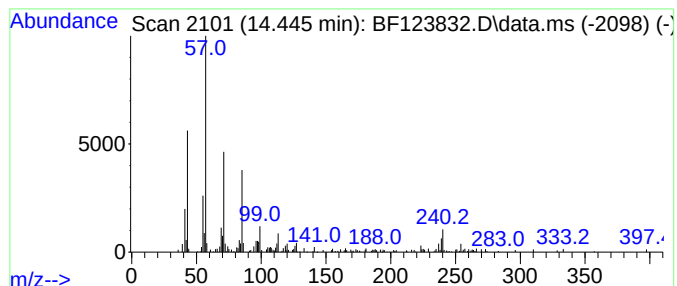
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	2.57 ng	180393	Chrysene-d12	13.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	92
2			Docosane	310	C22H46	000629-97-0	89
3			Hexadecane	226	C16H34	000544-76-3	76
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
5			Heptacosane	380	C27H56	000593-49-7	64



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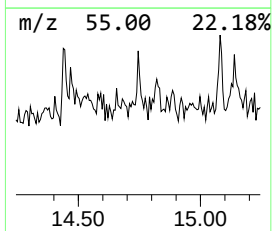
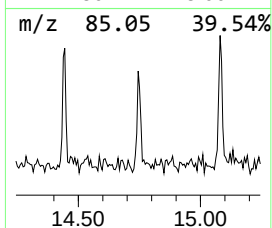
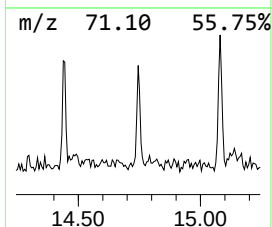
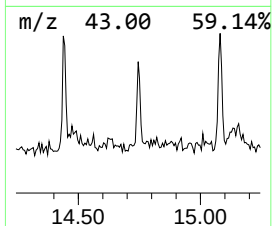
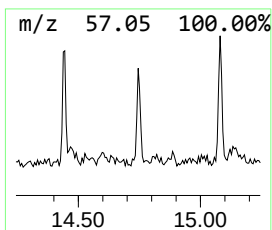
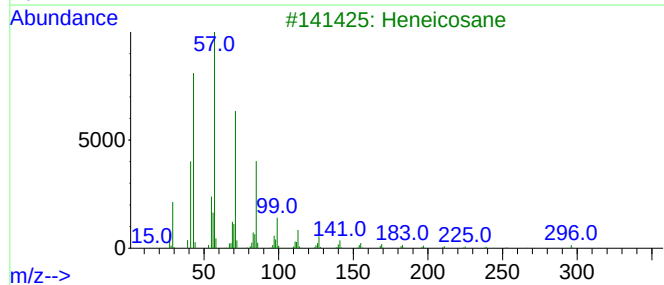
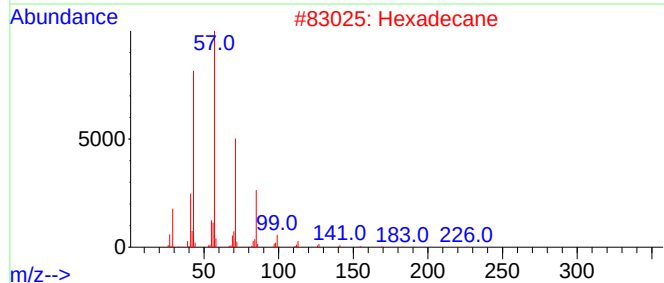
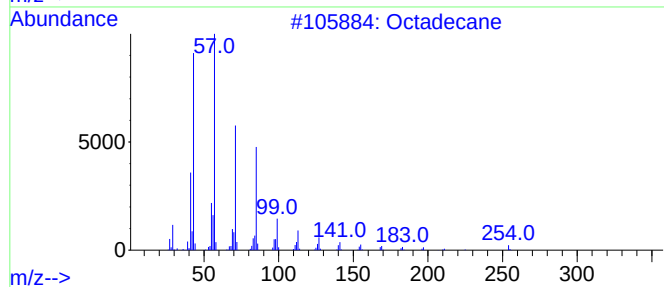
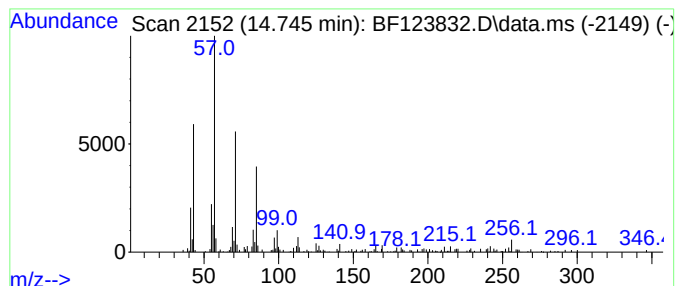
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	2.28 ng	139221	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	93
2			Hexadecane	226	C16H34	000544-76-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane	240	C17H36	000629-78-7	83
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123832.D
Acq On : 5 May 2021 17:36
Operator : JU/CG
Sample : M2279-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
EME-14

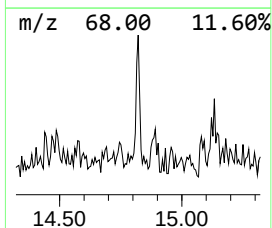
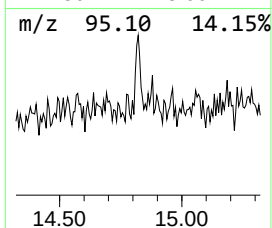
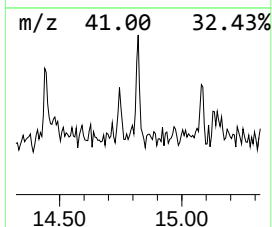
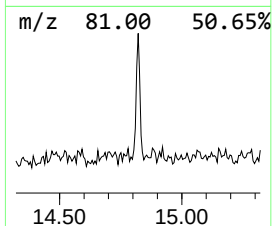
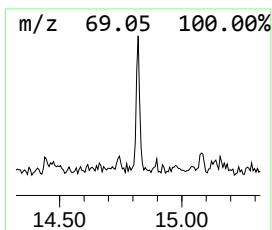
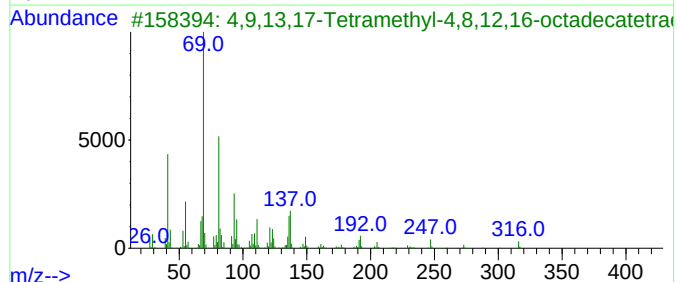
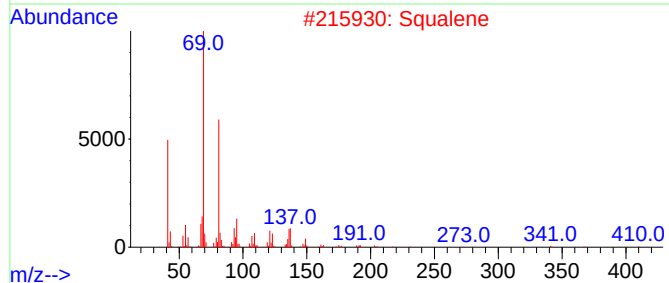
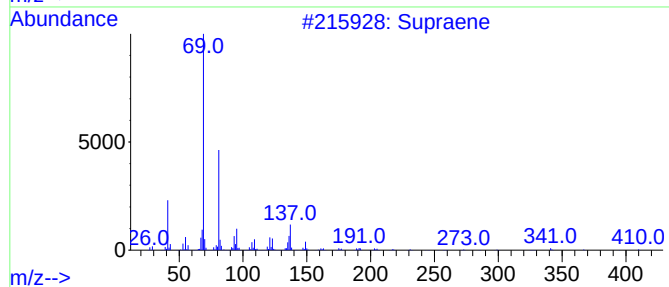
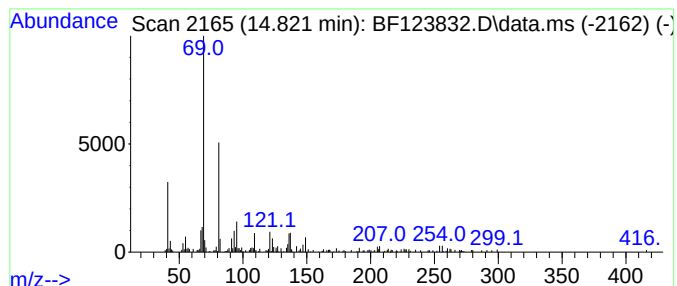
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.46 ng	150099	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	80
2			Squalene	410	C30H50	000111-02-4	80
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
4			.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123832.D
Acq On : 5 May 2021 17:36
Operator : JU/CG
Sample : M2279-03
Misc :
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Instrument :
BNA_F
ClientSampled :
EME-14

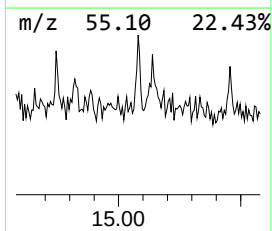
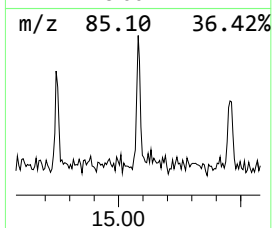
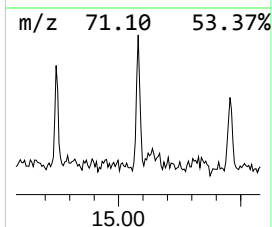
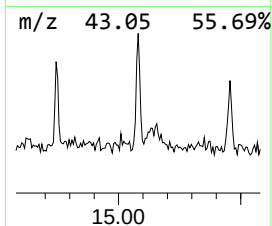
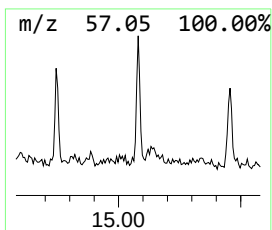
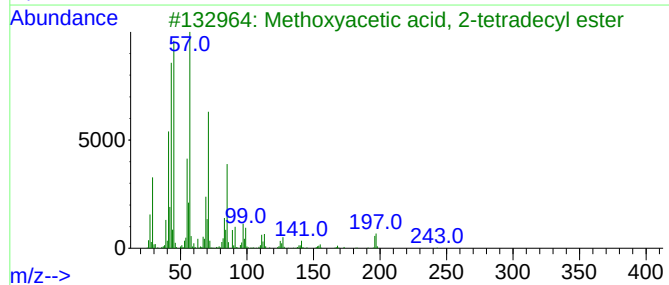
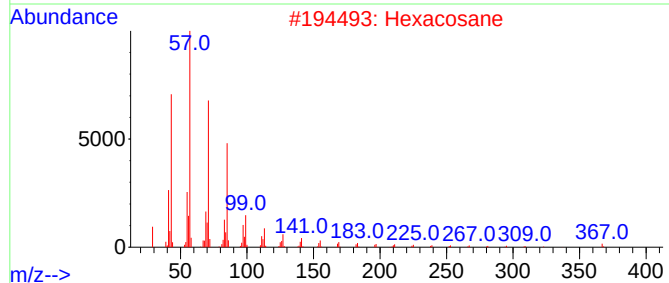
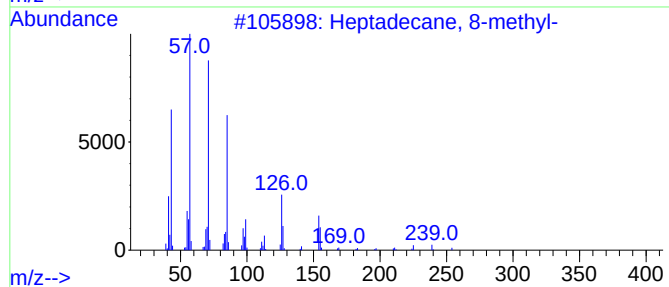
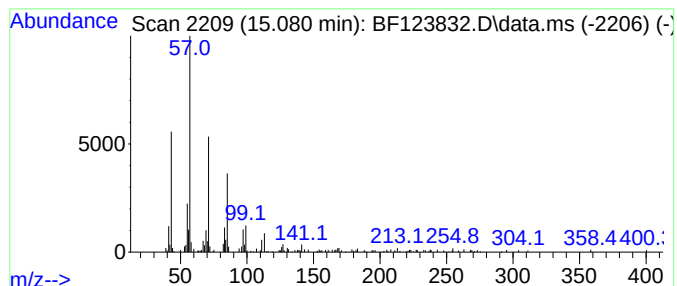
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane, 8-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	2.76 ng	168851	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 8-methyl-	254	C18H38	013287-23-5	81
2			Hexacosane	366	C26H54	000630-01-3	80
3			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	80
4			Hexadecane	226	C16H34	000544-76-3	72
5			Tritetracontane	605	C43H88	007098-21-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123832.D
Acq On : 5 May 2021 17:36
Operator : JU/CG
Sample : M2279-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

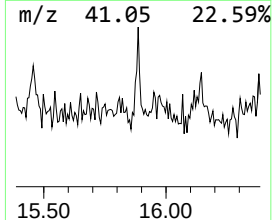
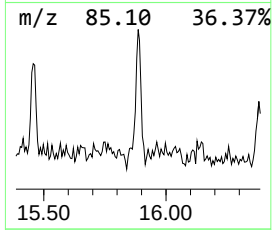
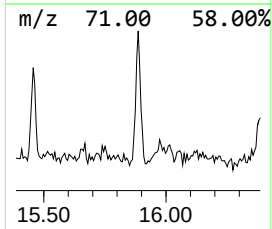
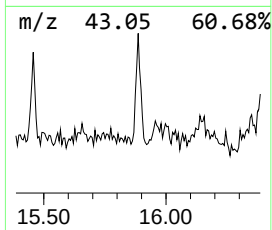
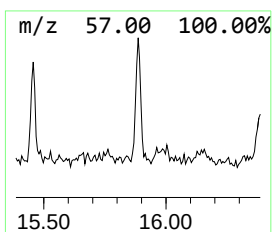
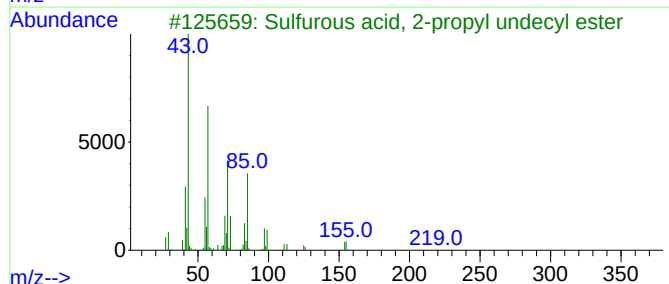
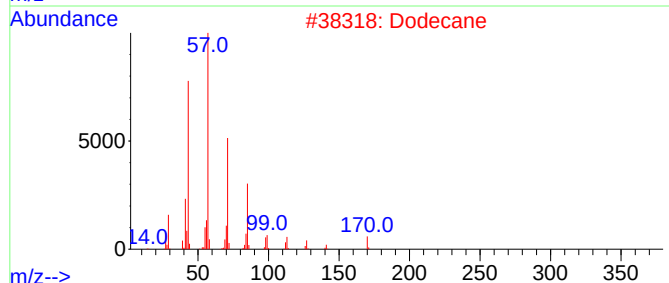
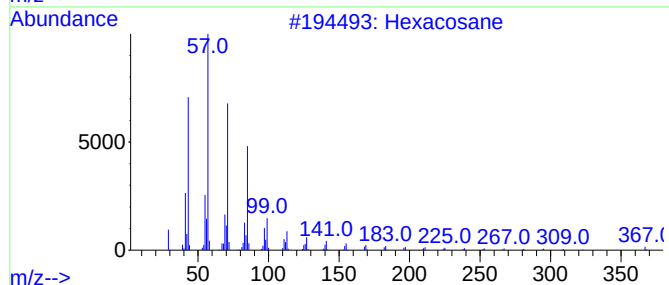
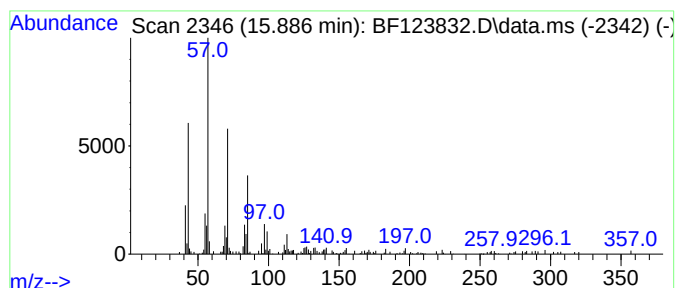
Instrument :
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ClientSampled :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.886	3.25 ng	198571	Perylene-d12		15.421	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	90
2	Dodecane		170	C12H26	000112-40-3	83
3	Sulfurous acid, 2-propyl undecyl...		278	C14H30O3S	1000309-12-2	80
4	Pentadecane		212	C15H32	000629-62-9	80
5	Heptacosane		380	C27H56	000593-49-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123832.D
Acq On : 5 May 2021 17:36
Operator : JU/CG
Sample : M2279-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

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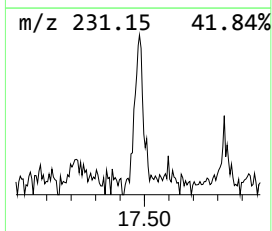
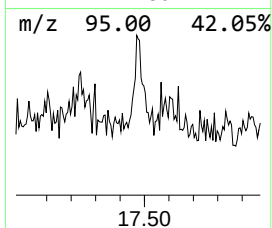
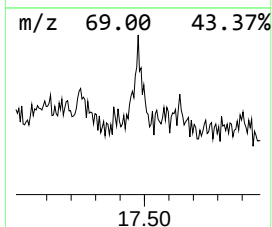
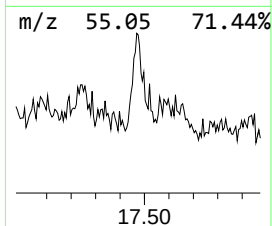
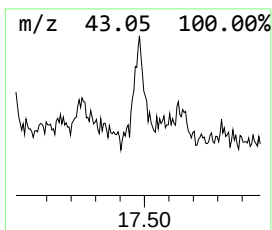
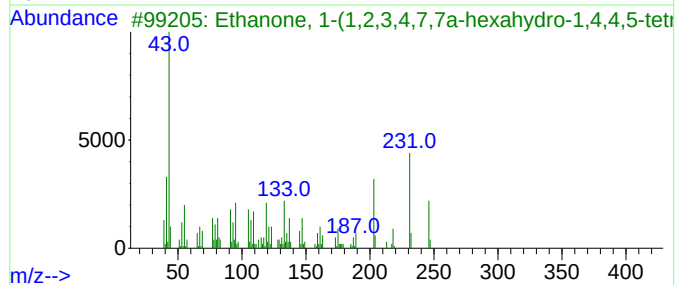
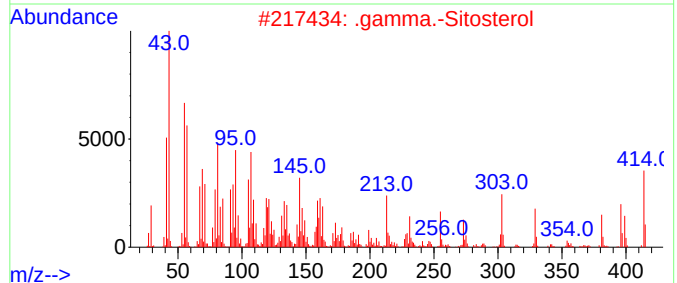
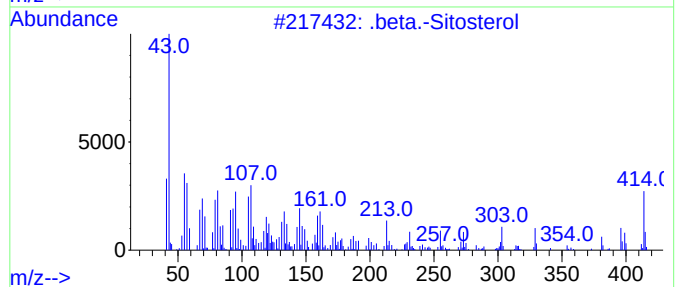
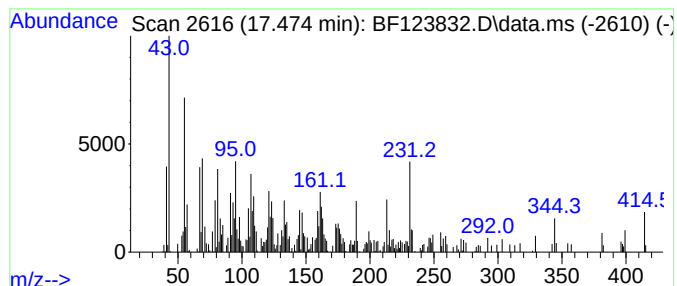
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 .beta.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.474	9.80 ng	598606	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.beta.-Sitosterol	414	C29H50O	000083-46-5	50
2	.		.gamma.-Sitosterol	414	C29H50O	000083-47-6	30
3	Ethanone, 1-(1,2,3,4,7,7a-hexahy...			246	C17H26O	032388-58-2	16
4	17-(1,5-Dimethylhexyl)-10,13-dim...			414	C29H50O	1000210-86-9	14
5	Stigmastan-3-en-6-ol			414	C29H50O	1000214-19-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123832.D
Acq On : 5 May 2021 17:36
Operator : JU/CG
Sample : M2279-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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4,4-Diallyl-cyc...	12.404	2.9	ng	263277	4	11.321	1846280	20.0
Octacosyl trifl...	13.821	8.5	ng	598168	5	13.962	1402470	20.0
Heneicosane	14.445	2.6	ng	180393	5	13.962	1402470	20.0
Octadecane	14.745	2.3	ng	139221	6	15.421	1221630	20.0
Supraene	14.821	2.5	ng	150099	6	15.421	1221630	20.0
Heptadecane, 8-...	15.080	2.8	ng	168851	6	15.421	1221630	20.0
Hexacosane	15.886	3.3	ng	198571	6	15.421	1221630	20.0
.beta.-Sitosterol	17.474	9.8	ng	598606	6	15.421	1221630	20.0