

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
 Data File : BF123833.D
 Acq On : 5 May 2021 18:07
 Operator : JU/CG
 Sample : M2279-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EME-15

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: BF123833.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	491	493	499	rVB	120183	135289	2.74%	0.330%
2	5.410	561	565	576	rBV	5336400	4772280	96.75%	11.643%
3	6.434	735	739	742	rBV	5674871	4932722	100.00%	12.035%
4	6.792	796	800	803	rBV	1927542	1411638	28.62%	3.444%
5	7.357	891	896	899	rBV	3960917	3207729	65.03%	7.826%
6	8.075	1013	1018	1022	rBV	2159129	1931462	39.16%	4.712%
7	9.157	1198	1202	1205	rBV	5870279	4691554	95.11%	11.446%
8	9.239	1213	1216	1220	rBV2	73056	69929	1.42%	0.171%
9	9.551	1266	1269	1272	rBV	288204	258031	5.23%	0.630%
10	9.833	1313	1317	1320	rVV	2500006	1966753	39.87%	4.798%
11	9.863	1320	1322	1326	rVB	93116	82764	1.68%	0.202%
12	10.039	1348	1352	1354	rBV2	60652	58452	1.18%	0.143%
13	10.380	1407	1410	1415	rBV	106781	92865	1.88%	0.227%
14	10.622	1447	1451	1455	rBV	3665884	3076684	62.37%	7.506%
15	10.745	1469	1472	1473	rBV	80843	82100	1.66%	0.200%
16	10.757	1473	1474	1477	rVV	108312	68955	1.40%	0.168%
17	10.810	1480	1483	1485	rBV	200918	185618	3.76%	0.453%
18	10.845	1485	1489	1492	rVV2	216026	273259	5.54%	0.667%
19	10.875	1492	1494	1496	rVV	209059	176958	3.59%	0.432%
20	10.898	1496	1498	1501	rVV2	170682	148001	3.00%	0.361%
21	10.933	1501	1504	1506	rVV4	86455	117185	2.38%	0.286%
22	10.986	1510	1513	1517	rVV3	161175	199795	4.05%	0.487%
23	11.027	1517	1520	1522	rVV	183124	189390	3.84%	0.462%
24	11.063	1525	1526	1531	rVB	108830	97501	1.98%	0.238%
25	11.216	1550	1552	1558	rVB4	72002	74294	1.51%	0.181%
26	11.322	1566	1570	1572	rBV	2202948	1786843	36.22%	4.359%
27	11.345	1572	1574	1577	rVV	564445	438396	8.89%	1.070%
28	11.392	1577	1582	1586	rVB	186667	213279	4.32%	0.520%
29	11.822	1652	1655	1657	rBV	93654	81764	1.66%	0.199%
30	11.851	1657	1660	1663	rVV2	192472	173259	3.51%	0.423%
31	11.933	1671	1674	1677	rBV	136593	149913	3.04%	0.366%
32	12.374	1746	1749	1751	rBV	63665	65706	1.33%	0.160%
33	12.404	1751	1754	1761	rVB5	128711	206833	4.19%	0.505%
34	12.533	1773	1776	1781	rVB	564634	461872	9.36%	1.127%
35	12.763	1808	1815	1818	rBV	521927	520983	10.56%	1.271%
36	12.792	1818	1820	1829	rVB4	109576	199015	4.03%	0.486%

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Integrator: RTE

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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 >

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37	12.910	1836	1840	1843	rBV	3990733	3229027	65.46%	7.878%
38	13.092	1869	1871	1874	rVB	93750	84963	1.72%	0.207%
39	13.157	1877	1882	1885	rBV2	96157	150192	3.04%	0.366%
40	13.492	1936	1939	1941	rBV2	61982	57168	1.16%	0.139%
41	13.827	1992	1996	2008	rVB3	247350	515129	10.44%	1.257%
42	13.963	2014	2019	2022	rBV2	1434576	1553554	31.49%	3.790%
43	13.992	2022	2024	2027	rVB	183885	155678	3.16%	0.380%
44	14.133	2046	2048	2051	rBV	91697	91866	1.86%	0.224%
45	14.445	2098	2101	2103	rBV2	157527	141320	2.86%	0.345%
46	14.745	2150	2152	2155	rVB	99518	79526	1.61%	0.194%
47	14.821	2162	2165	2169	rBV	117222	115806	2.35%	0.283%
48	14.998	2192	2195	2198	rBV	157321	209921	4.26%	0.512%
49	15.080	2206	2209	2212	rBV	159875	150410	3.05%	0.367%
50	15.357	2253	2256	2263	rVB	138875	156560	3.17%	0.382%
51	15.421	2263	2267	2271	rBV	925369	1150969	23.33%	2.808%
52	15.886	2342	2346	2352	rBV3	120438	194260	3.94%	0.474%
53	17.474	2612	2616	2628	rVB9	135389	352148	7.14%	0.859%

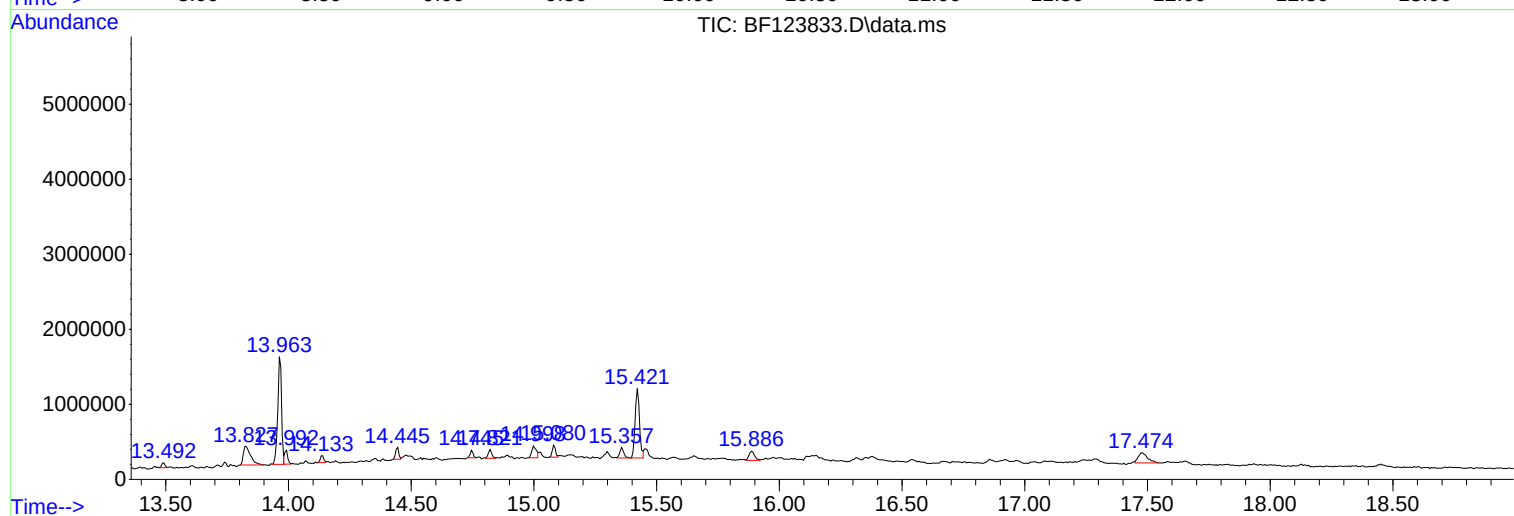
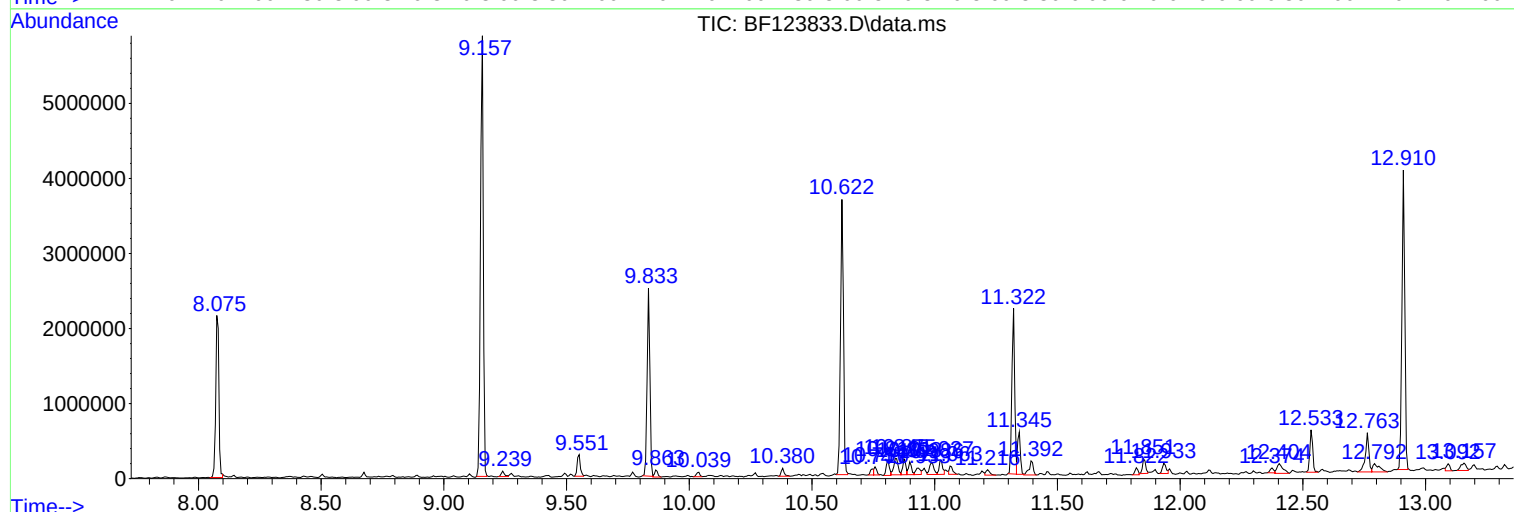
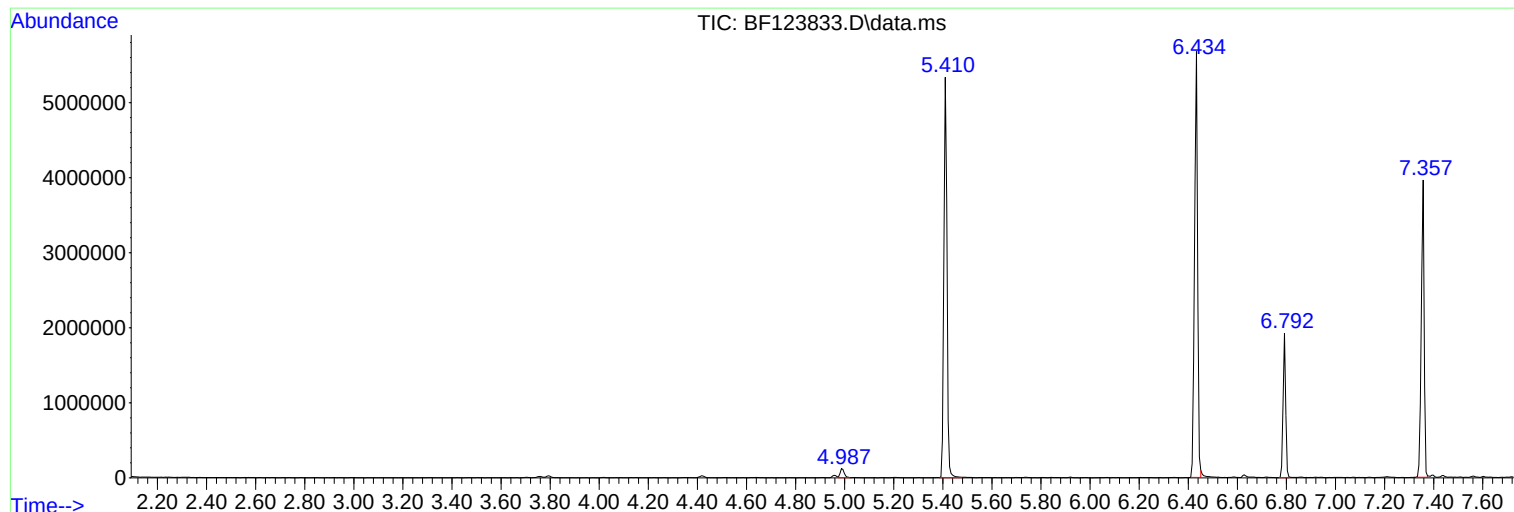
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : JU/CG
Sample : M2279-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

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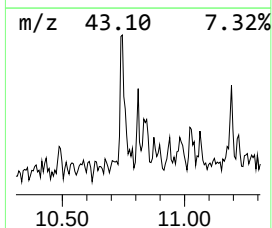
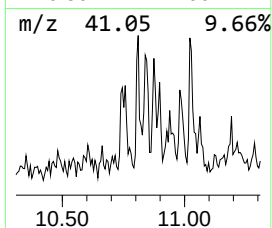
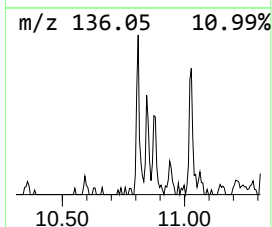
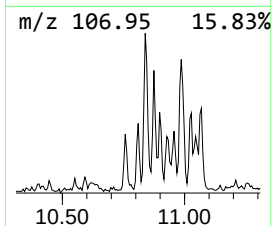
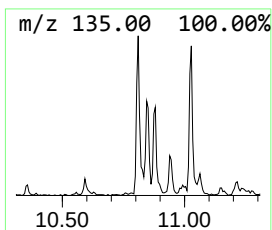
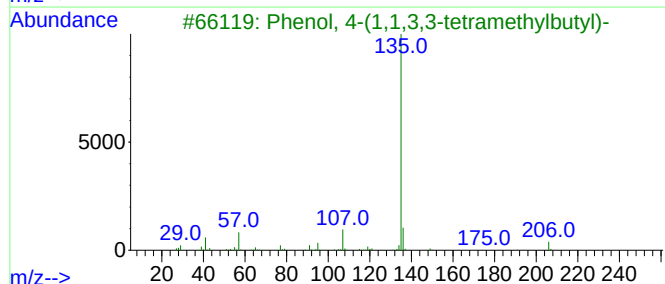
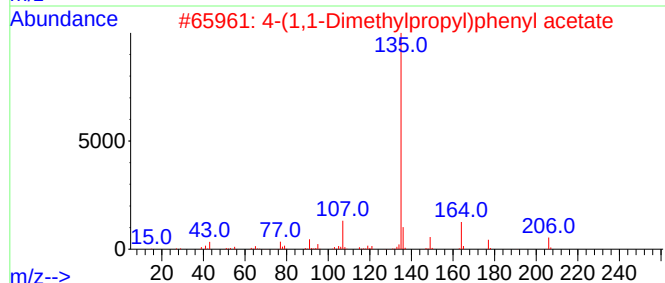
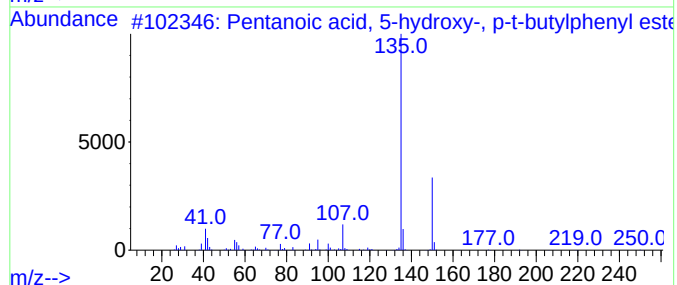
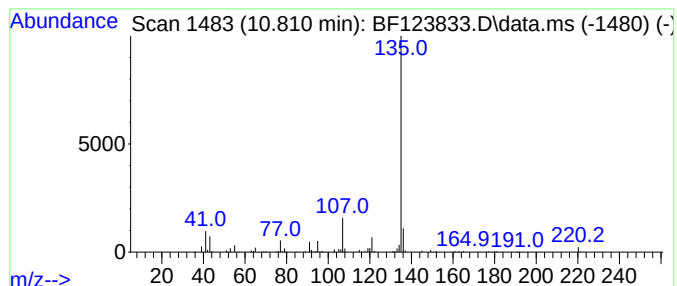
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentanoic acid, 5-hydroxy-,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.810	2.08 ng	185618	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 5-hydroxy-, p-t...	250	C15H22O3	166273-37-6	78
2			4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
3			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
4			Hexestrol	270	C18H22O2	000084-16-2	72
5			Hexestrol	270	C18H22O2	005635-50-7	72



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Instrument :
BNA_F
ClientSampled :
EME-15

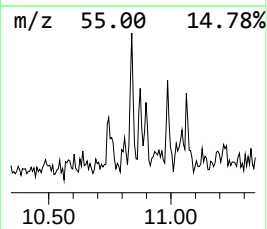
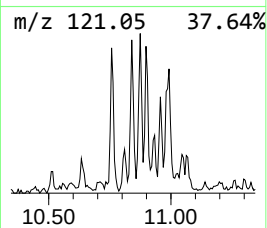
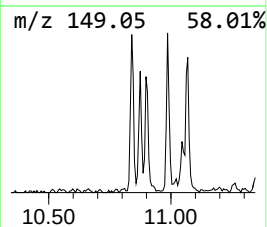
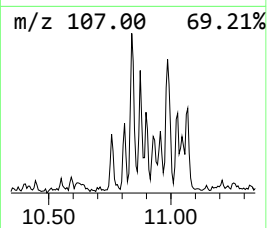
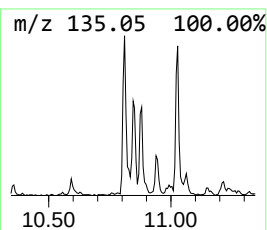
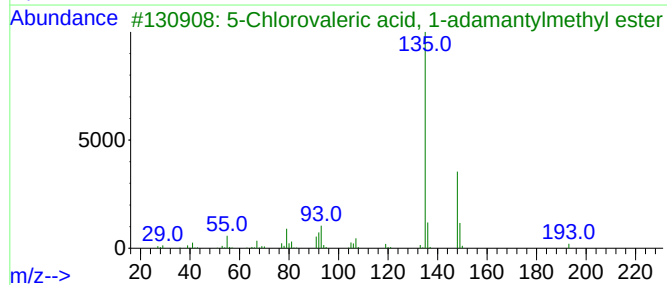
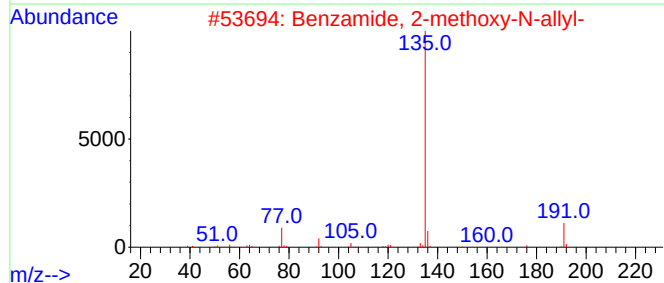
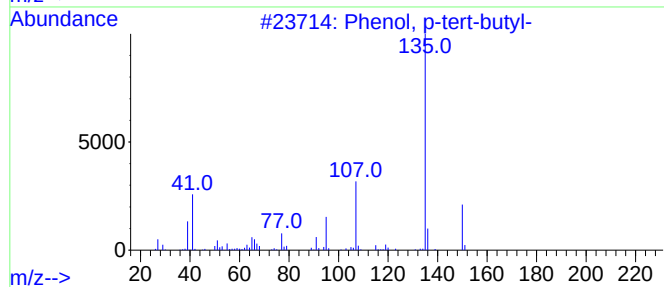
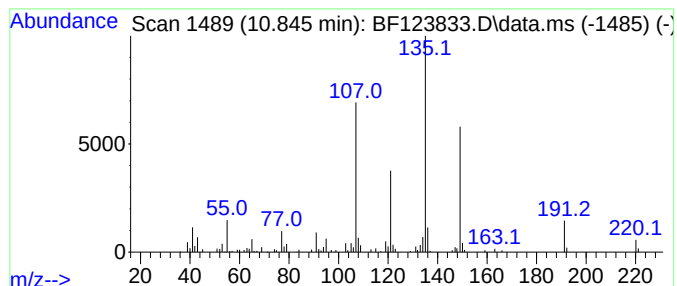
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Phenol, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	3.06 ng	273259	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	52
2			Benzamide, 2-methoxy-N-allyl-	191	C11H13NO2	1000339-10-5	43
3			5-Chlorovaleric acid, 1-adamanty...	284	C16H25ClO2	1000292-24-4	38
4			Heptafluorobutanoic acid, 1-adam...	362	C15H17F7O2	1000282-96-9	38
5			2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	38



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ALS Vial : 12 Sample Multiplier: 1

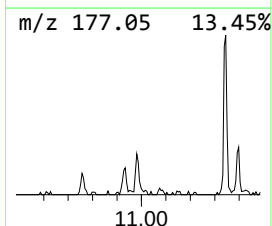
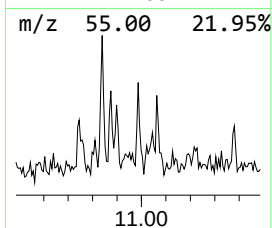
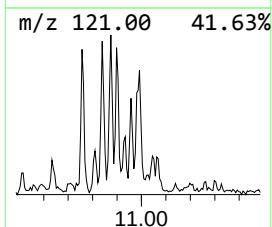
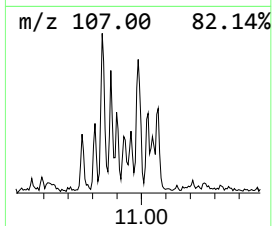
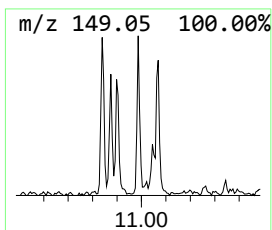
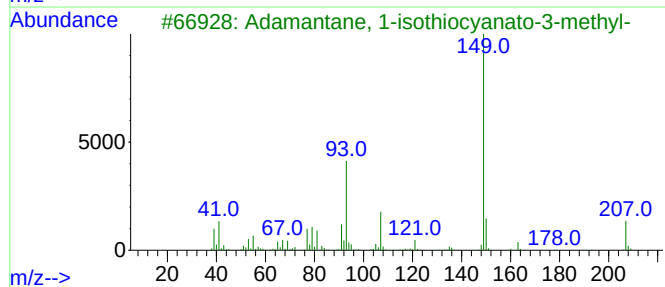
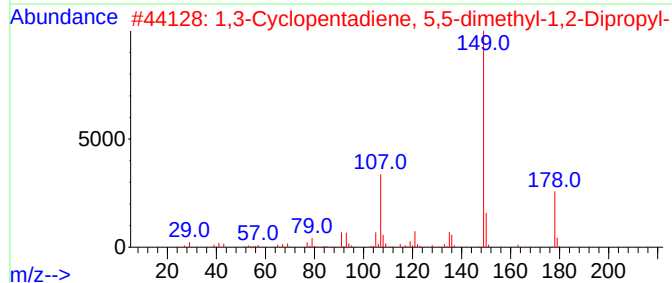
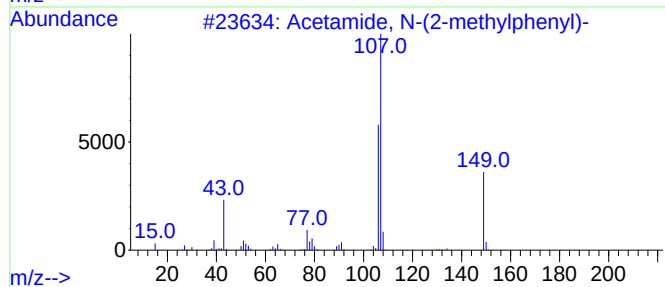
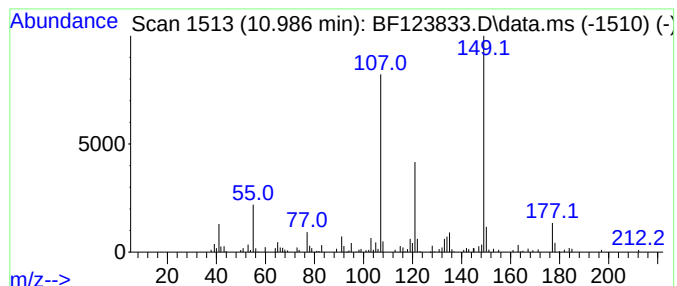
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Acetamide, N-(2-methylphenyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.986	2.24 ng	199795	Phenanthrene-d10		11.322	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Acetamide, N-(2-methylphenyl)-		149	C9H11NO	000120-66-1	64
2	1,3-Cyclopentadiene, 5,5-dimethy...		178	C13H22	1000163-88-0	50
3	Adamantane, 1-isothiocyanato-3-m...		207	C12H17NS	136860-48-5	38
4	Phenol, 2-methyl-4-(1,1,3,3-tetr...		220	C15H24O	002219-84-3	38
5	Diethyl Phthalate		222	C12H14O4	000084-66-2	38



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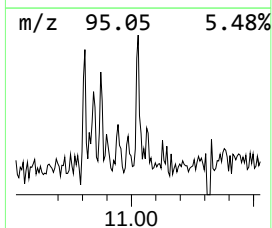
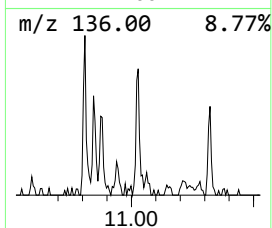
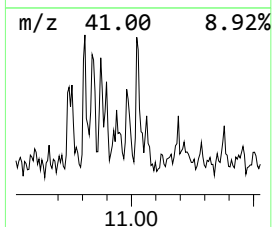
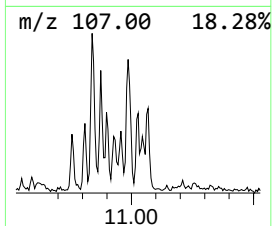
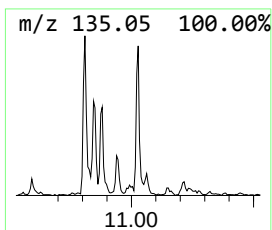
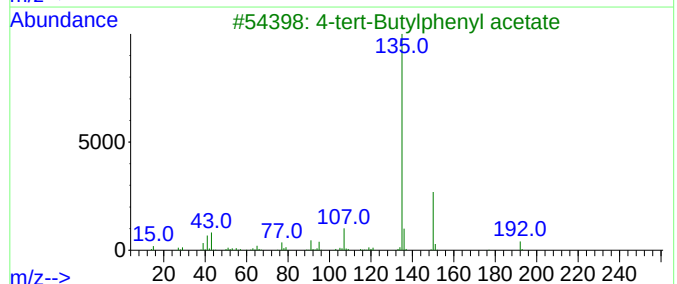
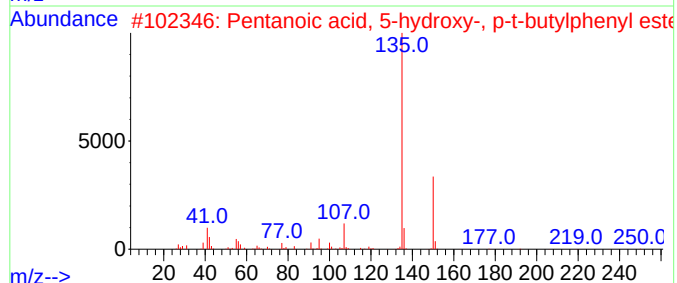
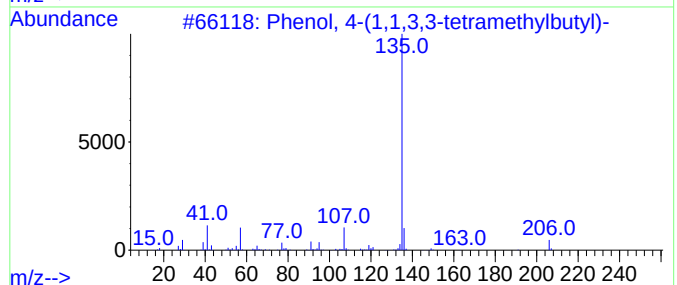
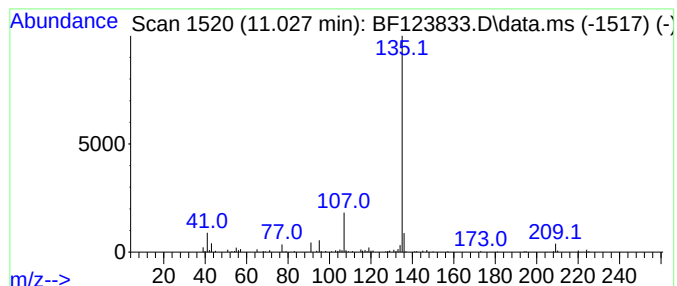
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.028	2.12 ng	189390	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	72
2			Pentanoic acid, 5-hydroxy-, p-t...	250	C15H22O3	166273-37-6	64
3			4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	56
4			((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	50
5			Benzeneacetonitrile, 2-fluoro-	135	C8H6FN	000326-62-5	50



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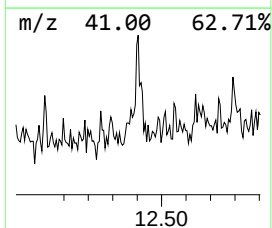
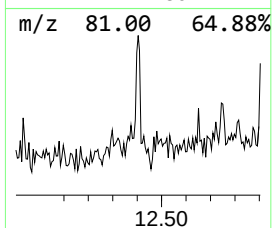
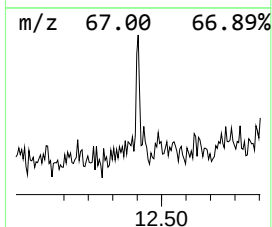
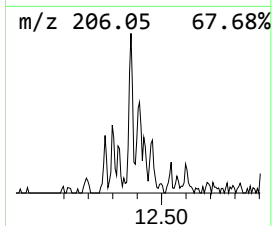
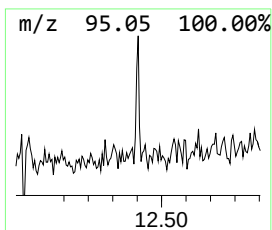
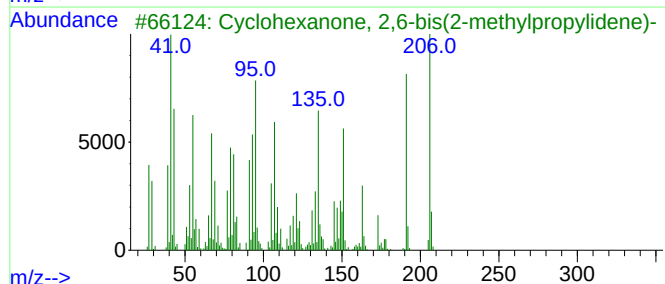
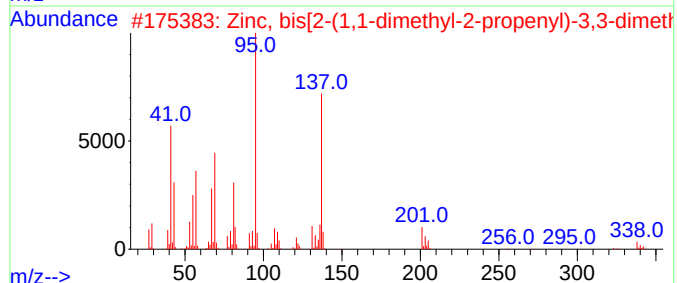
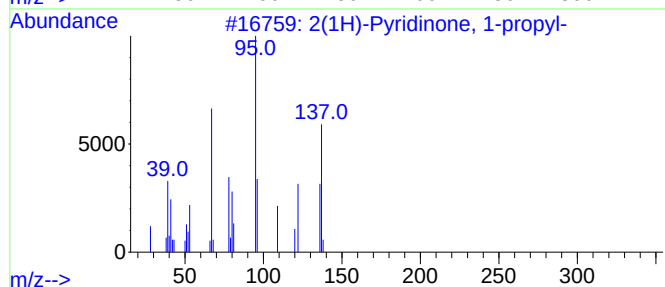
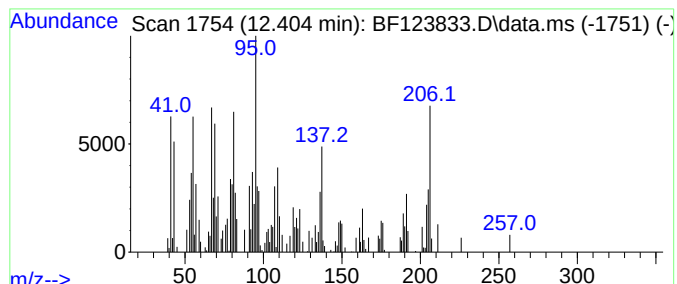
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2(1H)-Pyridinone, 1-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.404	2.32 ng	206833	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(1H)-Pyridinone, 1-propyl-	137	C8H11NO	019006-63-4	60
2			Zinc, bis[2-(1,1-dimethyl-2-prop...	338	C20H34Zn	074793-76-3	27
3			Cyclohexanone, 2,6-bis(2-methylp...	206	C14H22O	092368-82-6	25
4			2(E),4-Pentadienamide, N-[1-(dim...	206	C12H18N2O	075378-94-8	25
5			1-(2-Furyl)-4,4,4-trifluoro-1,3-...	206	C8H5F3O3	000326-90-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123833.D
Acq On : 5 May 2021 18:07
Operator : JU/CG
Sample : M2279-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-15

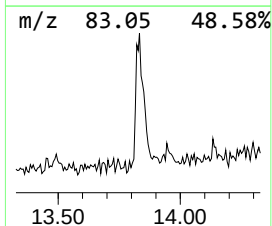
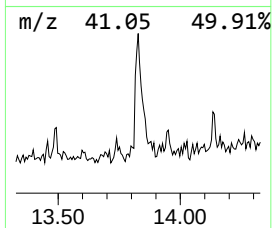
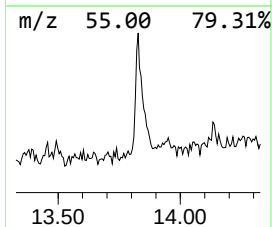
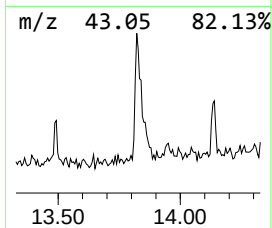
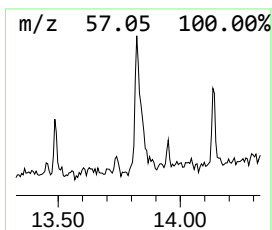
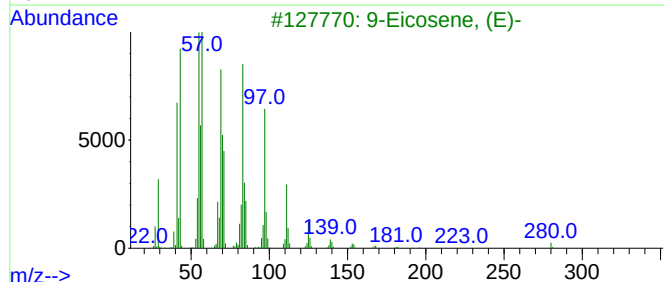
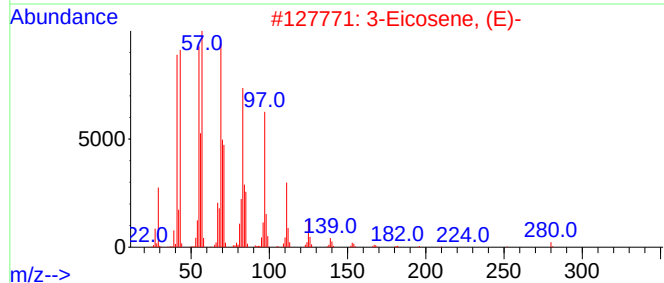
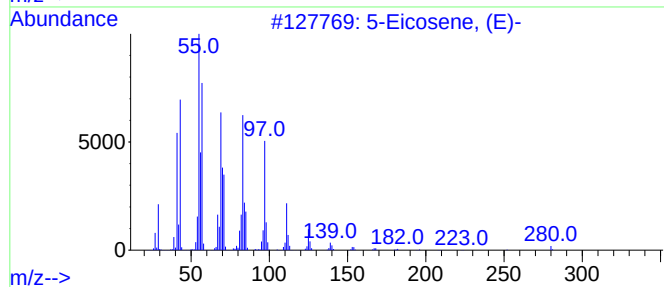
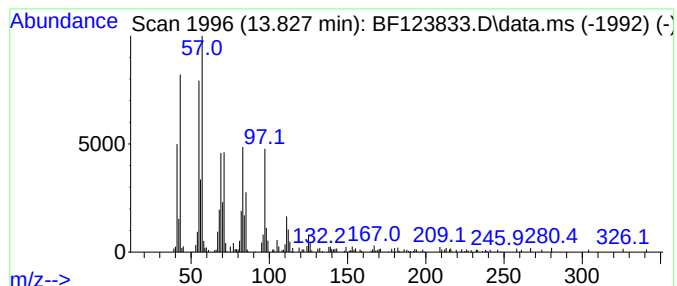
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	6.63 ng	515129	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	96
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	92
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	92
4			1-Heptadecene	238	C17H34	006765-39-5	90
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123833.D
Acq On : 5 May 2021 18:07
Operator : JU/CG
Sample : M2279-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
EME-15

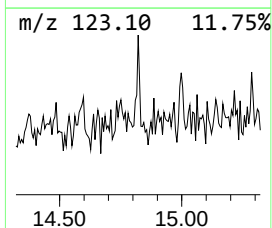
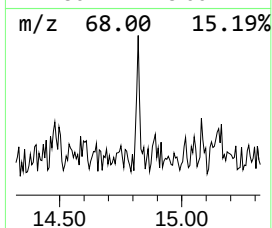
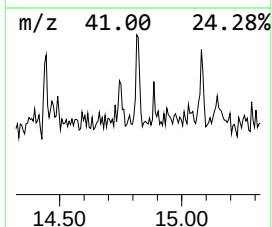
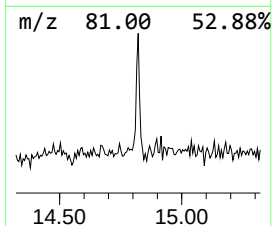
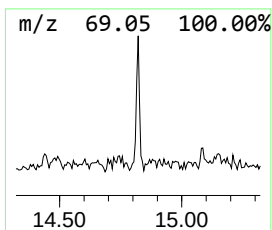
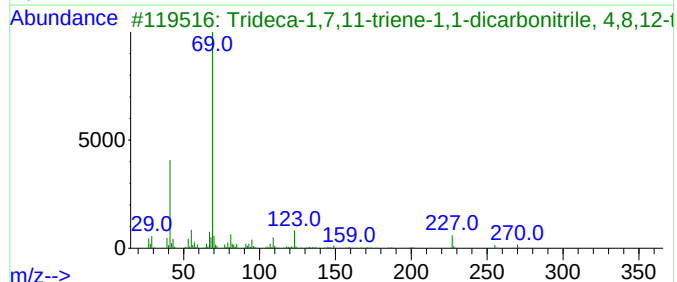
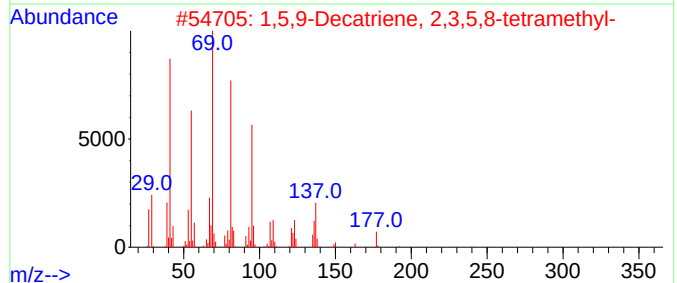
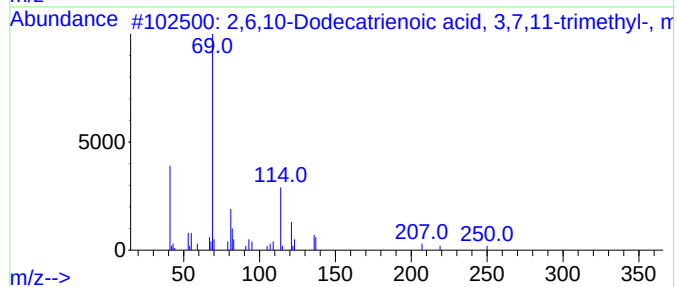
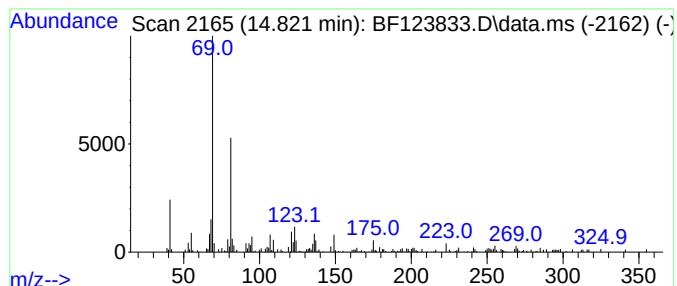
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,6,10-Dodecatrienoic acid,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.01 ng	115806	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	003675-00-1	72		
2	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72		
3	Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	64		
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64		
5	2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	004176-79-8	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123833.D
Acq On : 5 May 2021 18:07
Operator : JU/CG
Sample : M2279-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EME-15

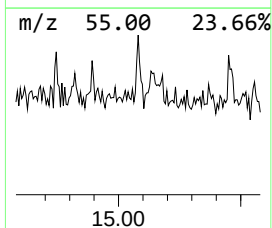
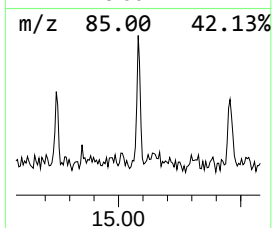
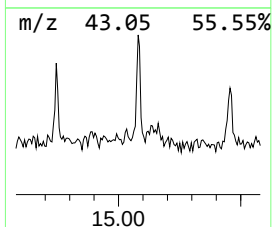
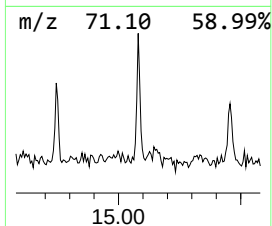
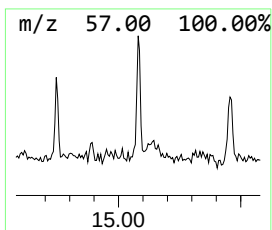
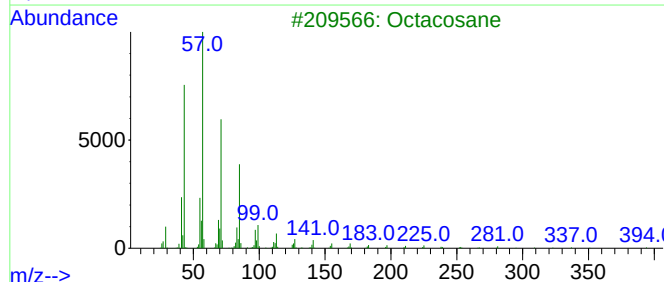
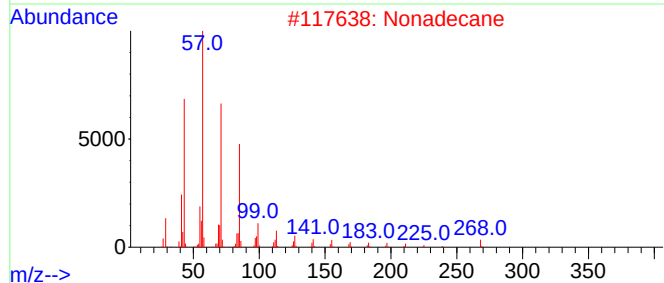
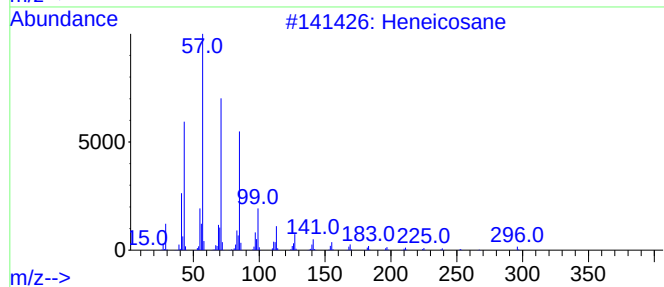
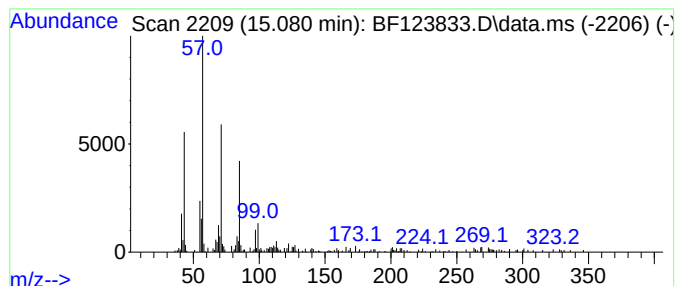
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	2.61 ng	150410	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	93
2			Nonadecane	268	C19H40	000629-92-5	89
3			Octacosane	394	C28H58	000630-02-4	86
4			Tridecane, 6-propyl-	226	C16H34	055045-10-8	83
5			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123833.D
Acq On : 5 May 2021 18:07
Operator : JU/CG
Sample : M2279-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-15

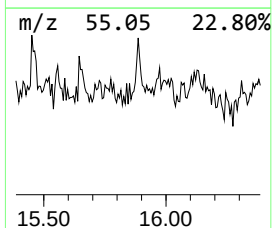
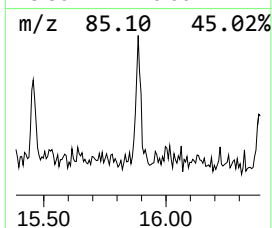
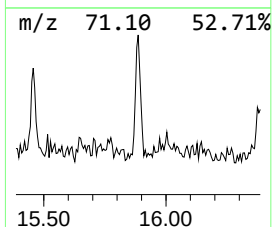
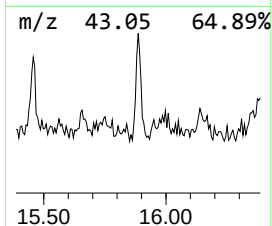
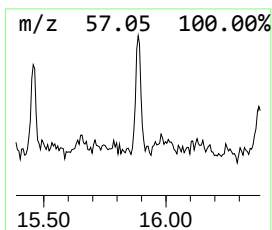
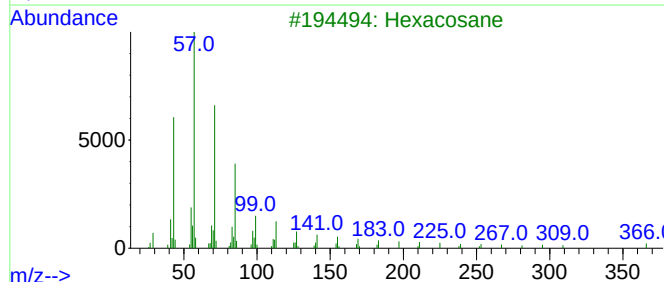
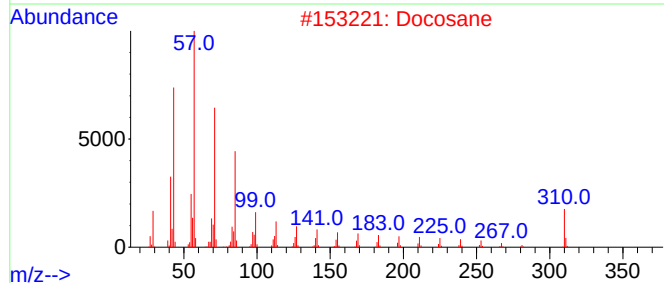
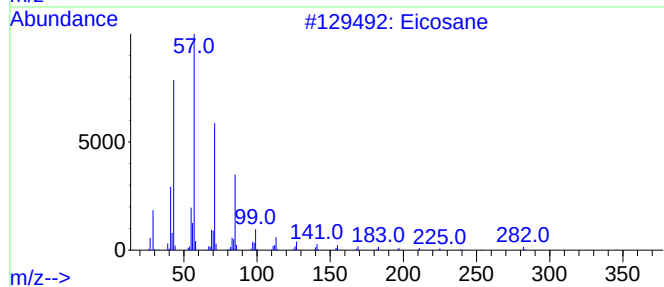
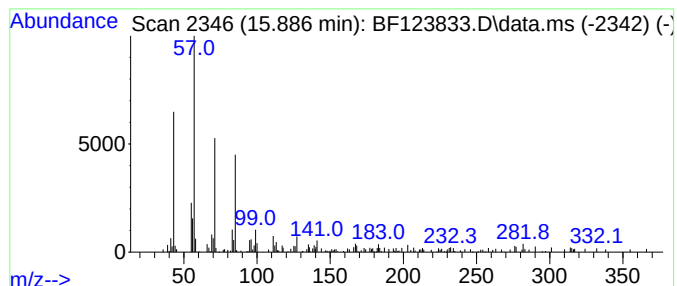
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	3.38 ng	194260	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	90
2	Docosane			310	C22H46	000629-97-0	87
3	Hexacosane			366	C26H54	000630-01-3	83
4	Tetracosane			338	C24H50	000646-31-1	83
5	Sulfurous acid, butyl decyl ester			278	C14H30O3S	1000309-17-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123833.D
Acq On : 5 May 2021 18:07
Operator : JU/CG
Sample : M2279-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
EME-15

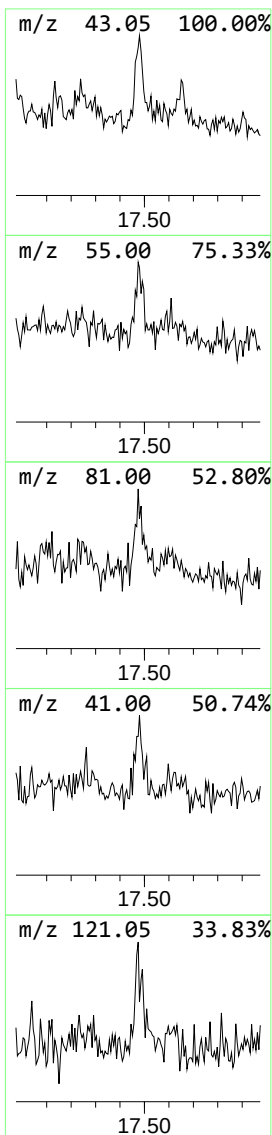
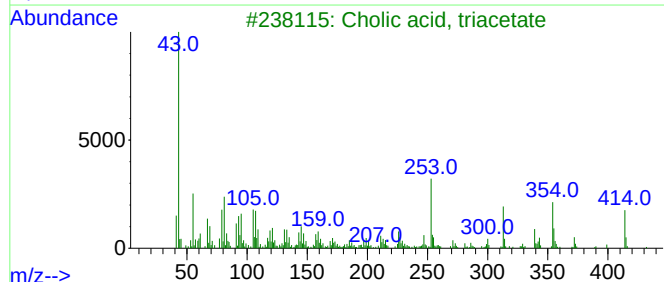
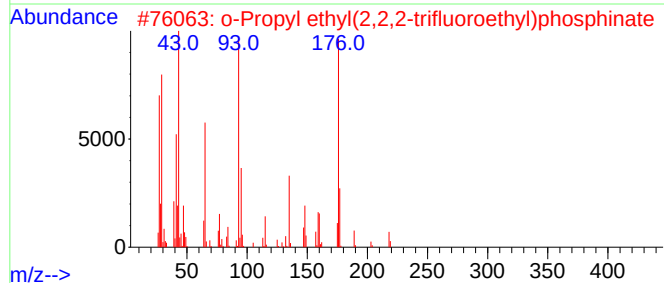
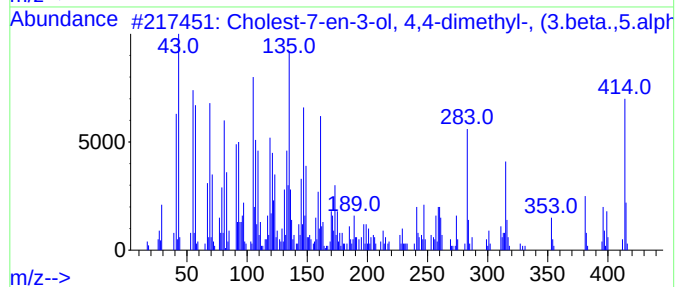
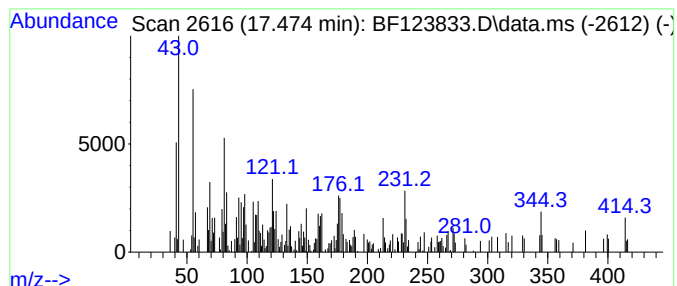
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.474	6.12 ng	352148	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholest-7-en-3-ol, 4,4-dimethyl-...	414	C29H50O	006384-28-7	18
2			o-Propyl ethyl(2,2,2-trifluoroet...	218	C7H14F3O2P	1000306-20-1	11
3			Cholic acid, triacetate	534	C30H46O8	052840-09-2	10
4			Phenol, 2-methoxy-4-(2-furfuryli...	231	C13H13NO3	105482-68-6	10
5			Stigmastan-7-one	414	C29H50O	055331-88-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123833.D
Acq On : 5 May 2021 18:07
Operator : JU/CG
Sample : M2279-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-15

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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Phenol, p-tert-...	10.845	3.1	ng	273259	4	11.322	1786840	20.0
Acetamide, N-(2...	10.986	2.2	ng	199795	4	11.322	1786840	20.0
Phenol, 4-(1,1,...	11.028	2.1	ng	189390	4	11.322	1786840	20.0
2(1H)-Pyridinon...	12.404	2.3	ng	206833	4	11.322	1786840	20.0
5-Eicosene, (E)-	13.827	6.6	ng	515129	5	13.963	1553550	20.0
2,6,10-Dodecatr...	14.821	2.0	ng	115806	6	15.421	1150970	20.0
Heneicosane	15.080	2.6	ng	150410	6	15.421	1150970	20.0
Eicosane	15.886	3.4	ng	194260	6	15.421	1150970	20.0
unknown17.47	17.474	6.1	ng	352148	6	15.421	1150970	20.0