

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
 Data File : BF123836.D
 Acq On : 5 May 2021 19:42
 Operator : JU/CG
 Sample : M2279-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EME-18

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: BF123836.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.998	492	495	502	rVB	48810	58666	1.09%	0.151%
2	5.416	562	566	569	rBV	5620370	5178651	96.65%	13.356%
3	6.434	735	739	742	rBV	5827867	5357901	100.00%	13.819%
4	6.792	796	800	803	rBV	1816762	1350527	25.21%	3.483%
5	7.357	891	896	899	rBV	4130456	3450331	64.40%	8.899%
6	8.075	1013	1018	1022	rBV	2018479	1799292	33.58%	4.641%
7	8.675	1117	1120	1122	rBV	81749	60337	1.13%	0.156%
8	9.157	1198	1202	1205	rBV	6059219	4723783	88.16%	12.183%
9	9.239	1213	1216	1220	rBV	108750	109770	2.05%	0.283%
10	9.492	1251	1259	1261	rBV6	46696	61073	1.14%	0.158%
11	9.551	1266	1269	1273	rBV	279395	294978	5.51%	0.761%
12	9.769	1304	1306	1310	rVB	95451	69786	1.30%	0.180%
13	9.833	1314	1317	1320	rVB	2340739	1750228	32.67%	4.514%
14	10.269	1388	1391	1394	rVB	98185	70932	1.32%	0.183%
15	10.381	1407	1410	1416	rBV3	40921	61186	1.14%	0.158%
16	10.622	1447	1451	1455	rBV	3475972	2956255	55.18%	7.625%
17	10.745	1468	1472	1476	rBV	131497	151074	2.82%	0.390%
18	11.222	1550	1553	1557	rVB3	49550	59747	1.12%	0.154%
19	11.322	1566	1570	1572	rBV	1831690	1505941	28.11%	3.884%
20	11.345	1572	1574	1577	rVV	276503	214512	4.00%	0.553%
21	11.392	1581	1582	1585	rVB	91753	60678	1.13%	0.156%
22	11.857	1658	1661	1666	rBV2	274872	286786	5.35%	0.740%
23	11.933	1671	1674	1677	rBV2	85841	85006	1.59%	0.219%
24	12.404	1751	1754	1761	rVB5	127542	205871	3.84%	0.531%
25	12.533	1773	1776	1779	rVB	316518	259859	4.85%	0.670%
26	12.763	1810	1815	1818	rBV	337140	335787	6.27%	0.866%
27	12.910	1836	1840	1844	rBV	3782725	3126984	58.36%	8.065%
28	13.092	1869	1871	1874	rVB2	69985	60774	1.13%	0.157%
29	13.145	1877	1880	1885	rVV3	103399	137922	2.57%	0.356%
30	13.321	1907	1910	1913	rBV2	68636	68056	1.27%	0.176%
31	13.492	1936	1939	1941	rBV	92685	85581	1.60%	0.221%
32	13.821	1992	1995	2009	rVB2	396886	781036	14.58%	2.014%
33	13.963	2015	2019	2022	rBV	1242536	1296676	24.20%	3.344%
34	13.992	2022	2024	2029	rVB	133758	117566	2.19%	0.303%
35	14.133	2046	2048	2051	rVB	137961	119456	2.23%	0.308%
36	14.439	2098	2100	2103	rBV	197509	186164	3.47%	0.480%

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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

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

37	14.745	2150	2152	2155	rVB	159475	131958	2.46%	0.340%
38	14.821	2162	2165	2169	rVB	149345	135883	2.54%	0.350%
39	14.998	2193	2195	2204	rVB2	120002	221304	4.13%	0.571%
40	15.080	2206	2209	2212	rVV2	177856	178811	3.34%	0.461%
41	15.421	2263	2267	2270	rBV	749922	864857	16.14%	2.231%
42	15.457	2270	2273	2278	rVB2	142399	196325	3.66%	0.506%
43	15.886	2342	2346	2351	rBV	128789	177880	3.32%	0.459%
44	17.480	2612	2617	2627	rVB	142674	366783	6.85%	0.946%

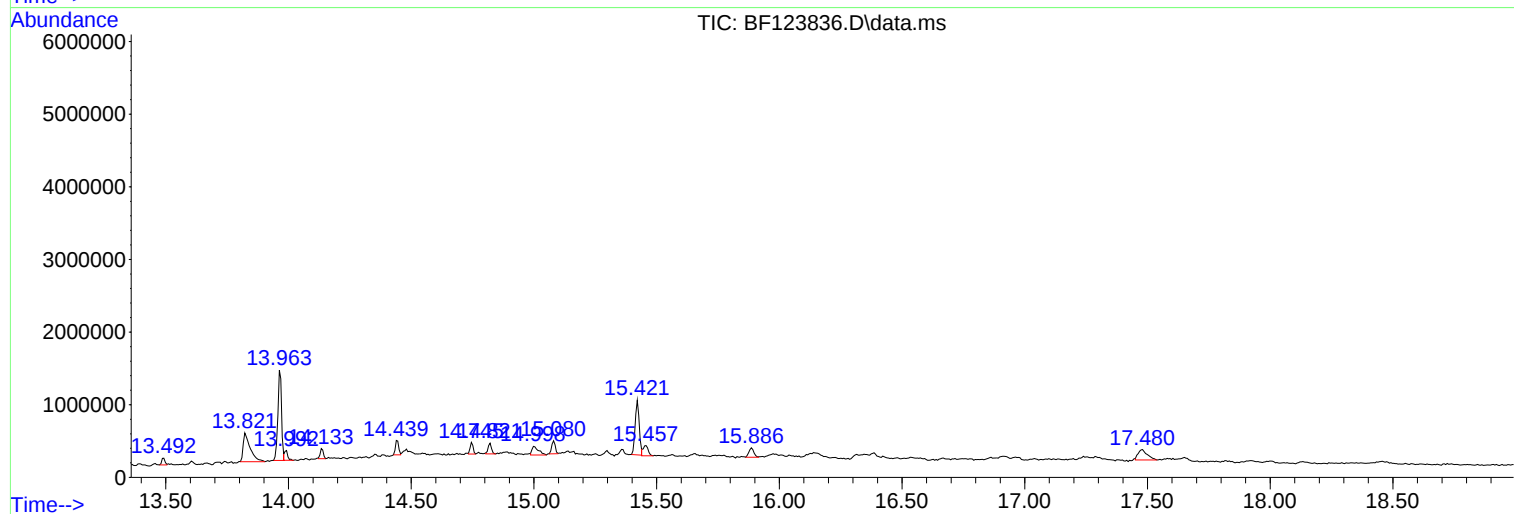
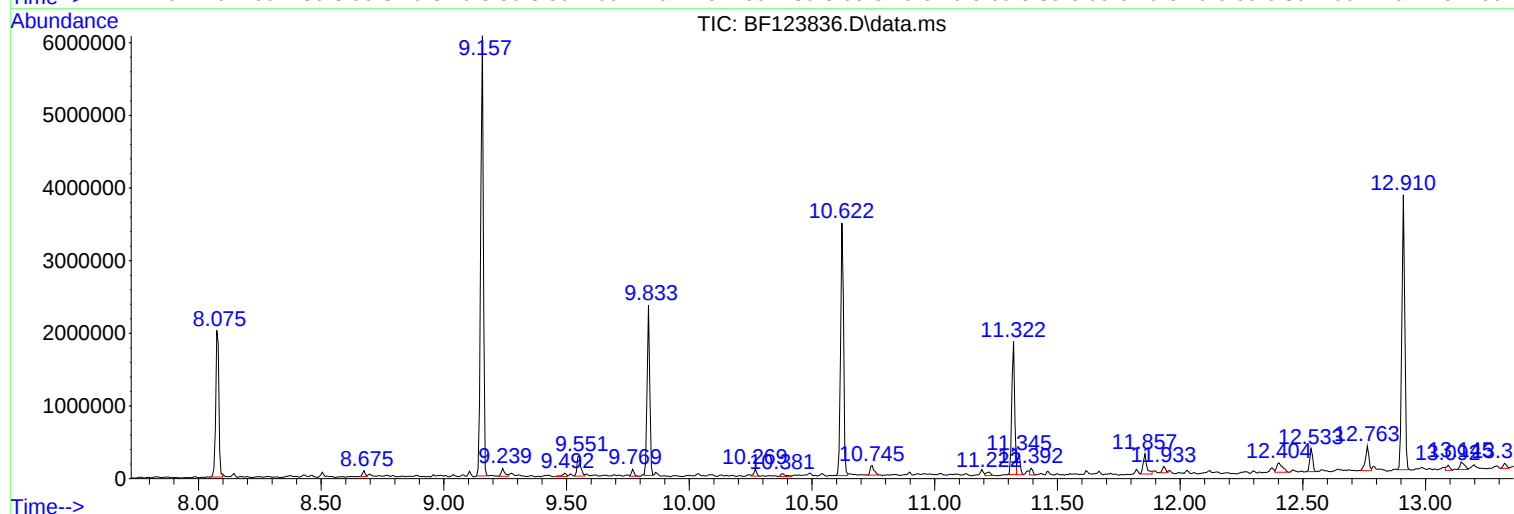
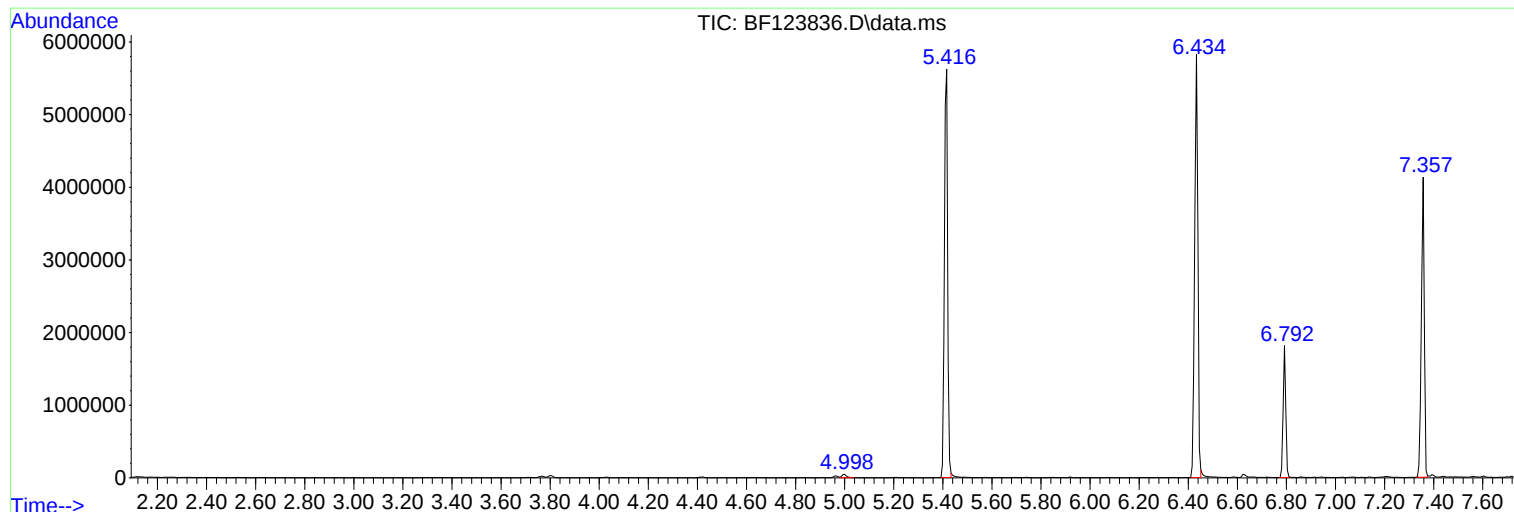
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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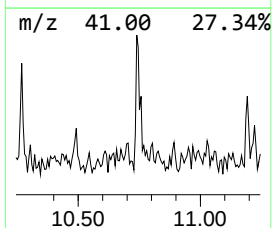
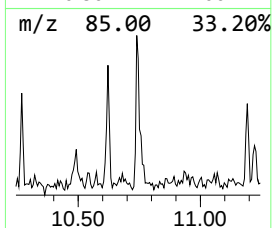
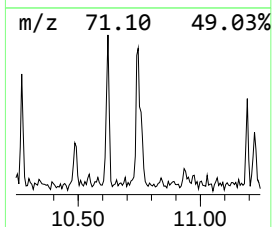
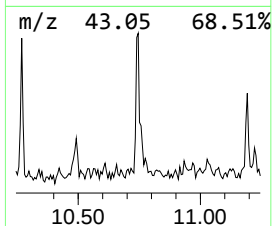
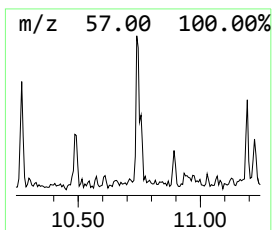
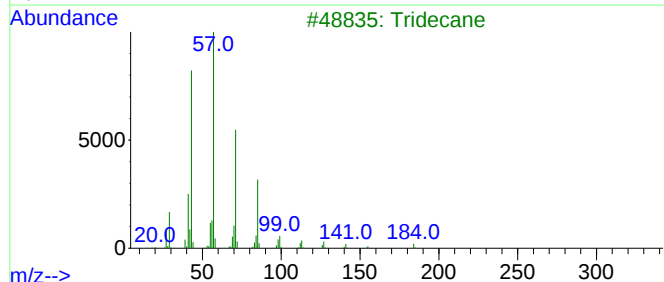
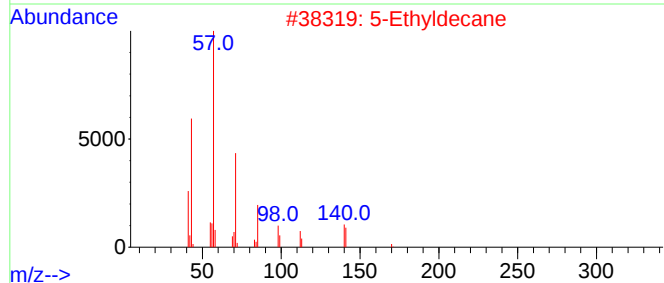
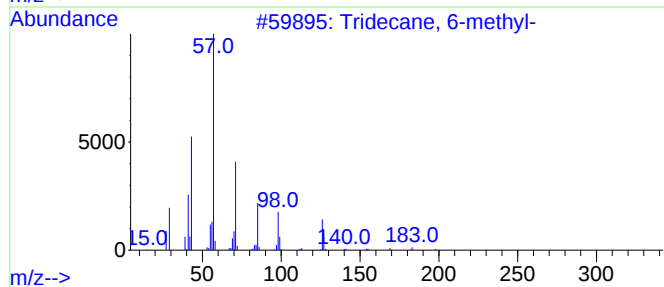
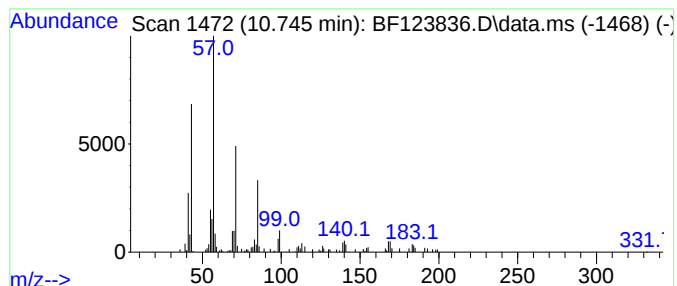
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tridecane, 6-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	2.01 ng	151074	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 6-methyl-	198	C14H30	013287-21-3	83
2			5-Ethyldecane	170	C12H26	017302-36-2	83
3			Tridecane	184	C13H28	000629-50-5	83
4			Dodecane, 2,5-dimethyl-	198	C14H30	056292-65-0	80
5			Heptacosane	380	C27H56	000593-49-7	72



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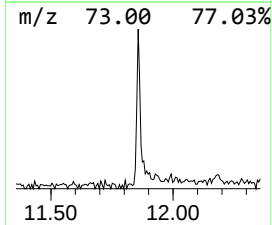
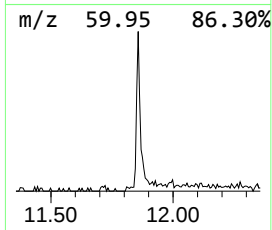
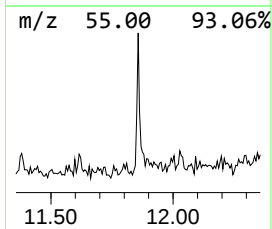
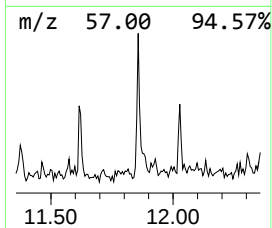
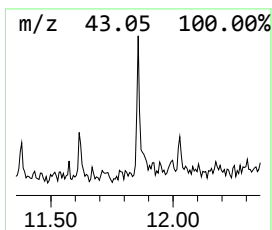
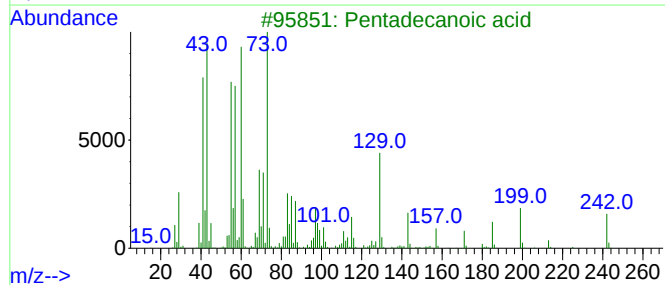
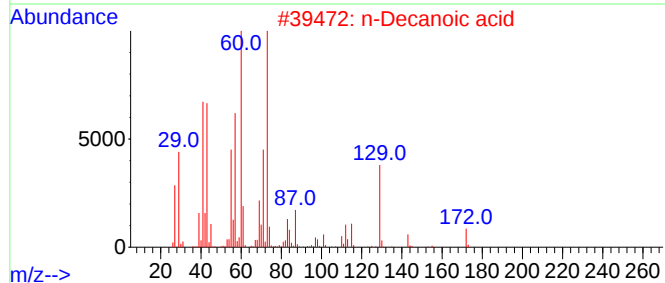
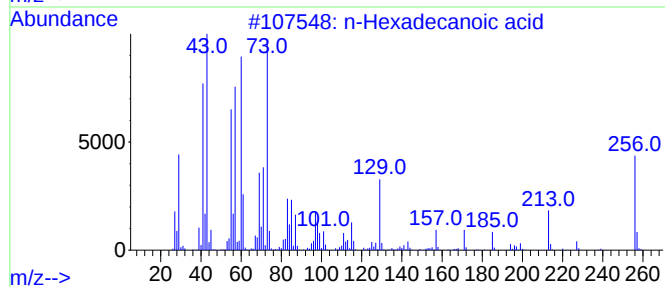
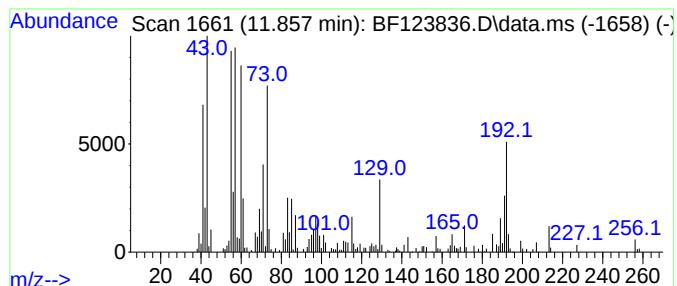
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	3.81 ng	286786	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2			n-Decanoic acid	172	C10H20O2	000334-48-5	60
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	50
5			Dodecanoic acid	200	C12H24O2	000143-07-7	49



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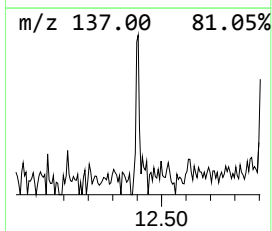
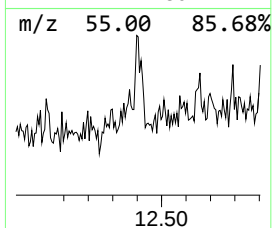
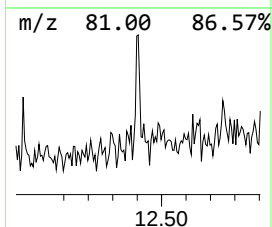
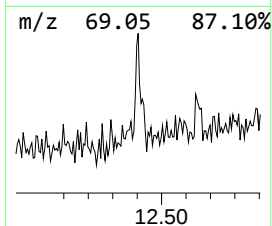
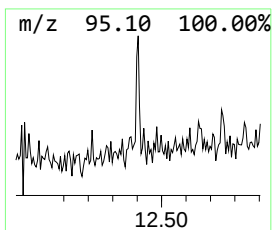
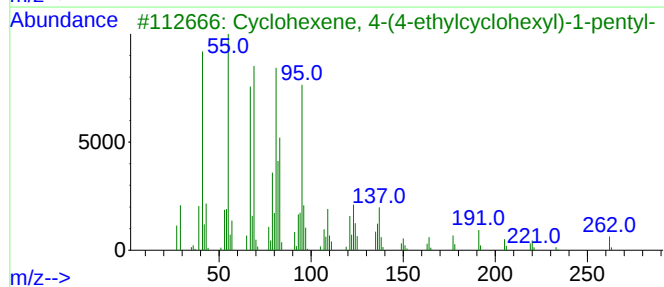
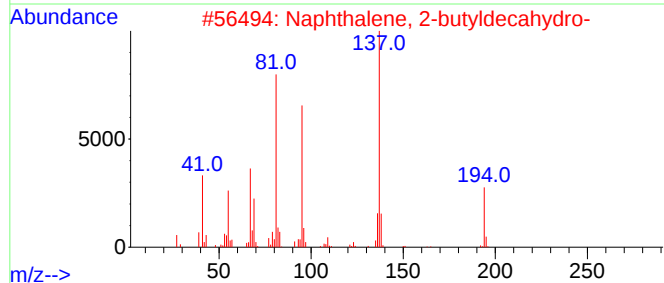
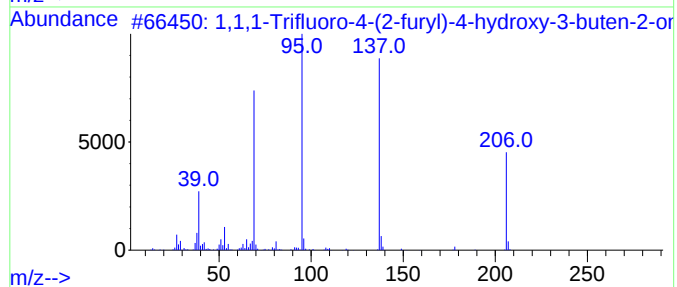
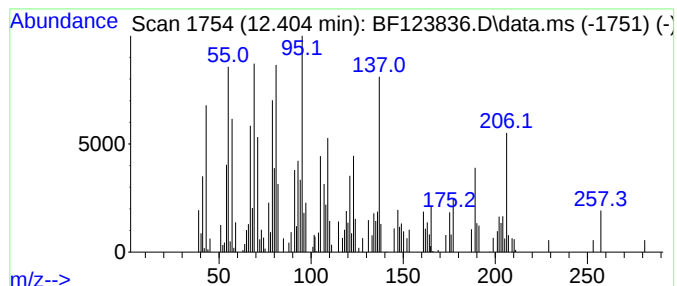
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.404 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.404	2.73 ng	205871	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1-Trifluoro-4-(2-furyl)-4-hy...	206	C8H5F3O3	015788-03-1	38		
2	Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	35		
3	Cyclohexene, 4-(4-ethylcyclohexy...	262	C19H34	301643-32-3	27		
4	Acetic acid, 3-(5,5-dimethyl-spi...	250	C16H26O2	077143-33-0	27		
5	2-Bromomethyl-1-isopropenyl-3-me...	216	C10H17Br	1000187-07-8	27		



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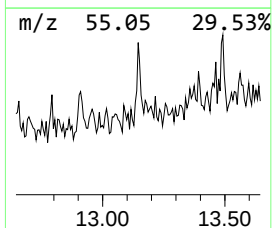
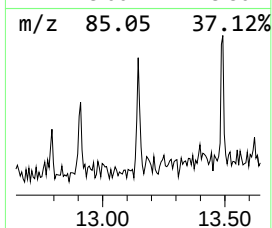
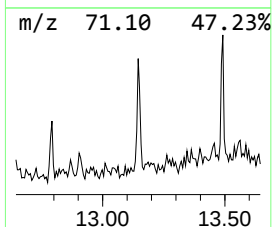
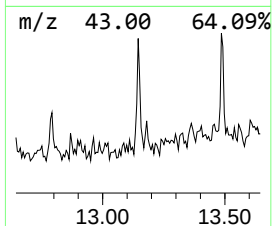
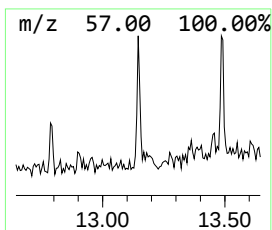
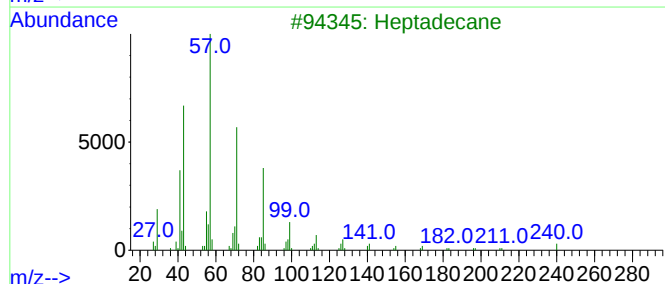
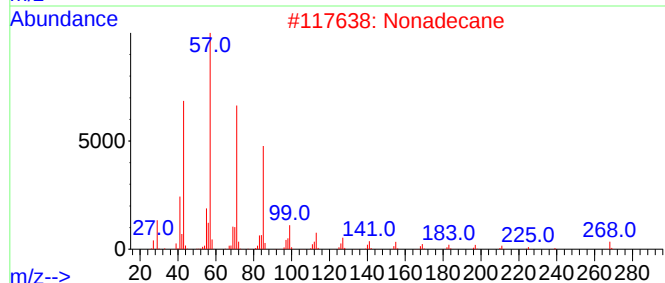
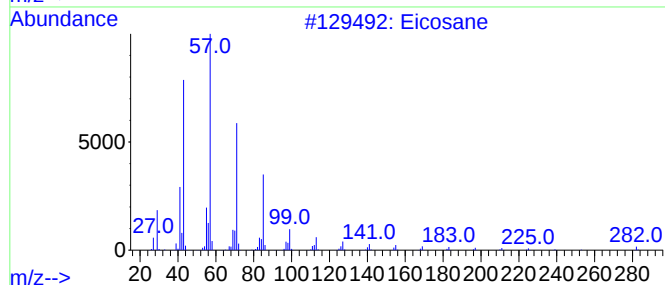
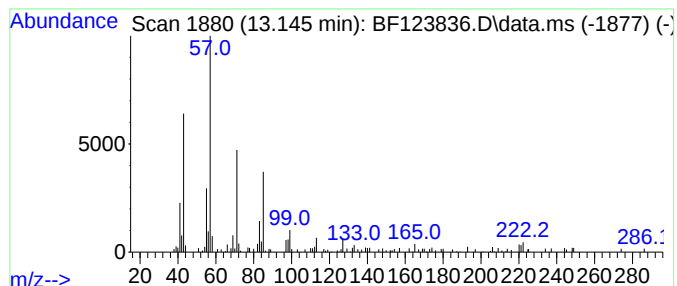
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.145	2.13 ng	137922	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	74
2	Nonadecane			268	C19H40	000629-92-5	72
3	Heptadecane			240	C17H36	000629-78-7	72
4	Heptacosane, 1-chloro-			414	C27H55Cl	062016-79-9	72
5	2-Bromo dodecane			248	C12H25Br	013187-99-0	72



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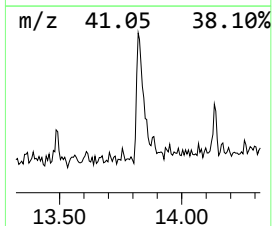
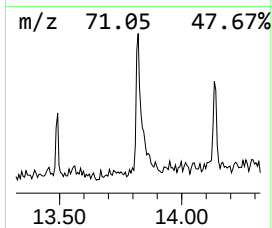
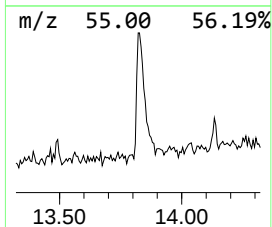
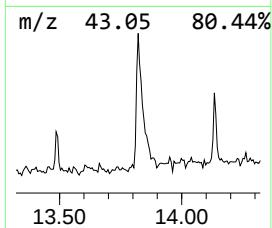
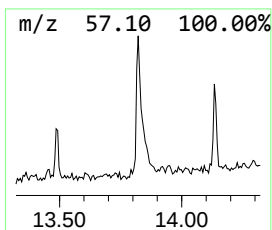
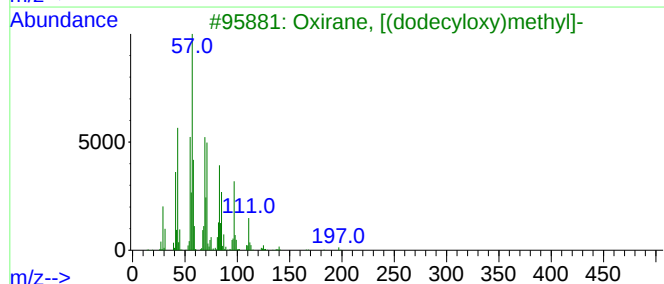
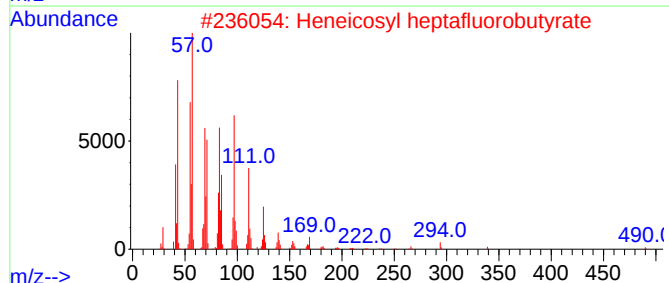
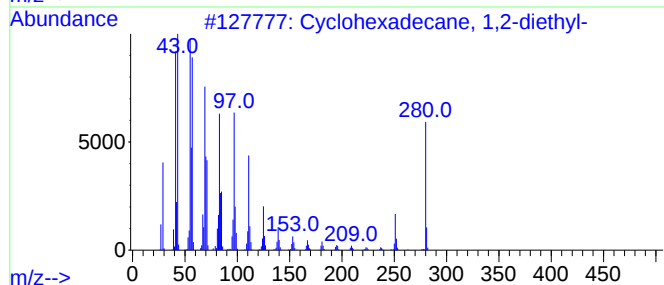
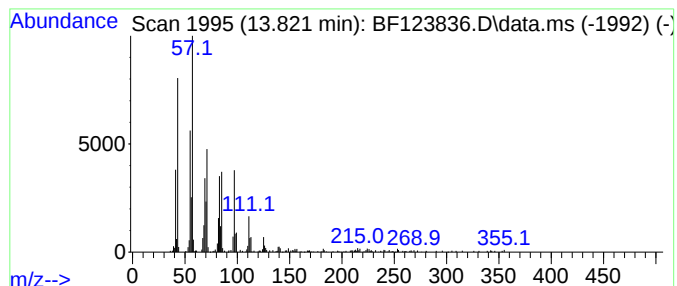
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclohexadecane, 1,2-diethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	12.05 ng	781036	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	93
2			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
3			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	91
4			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123836.D
Acq On : 5 May 2021 19:42
Operator : JU/CG
Sample : M2279-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

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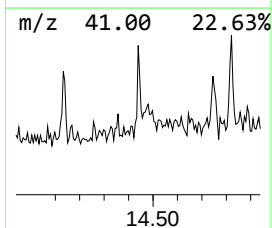
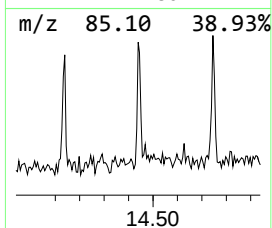
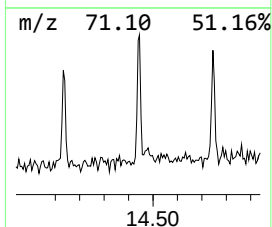
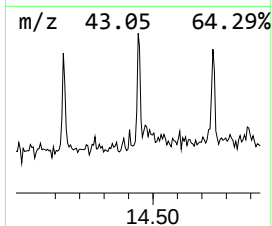
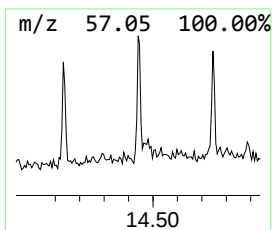
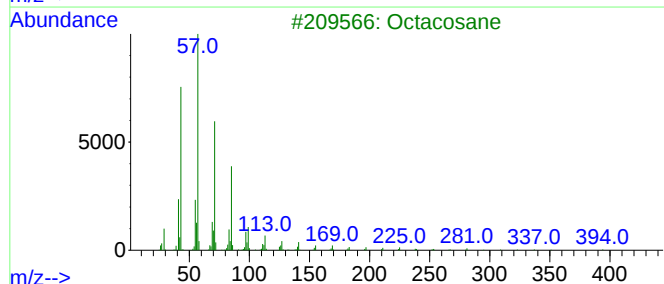
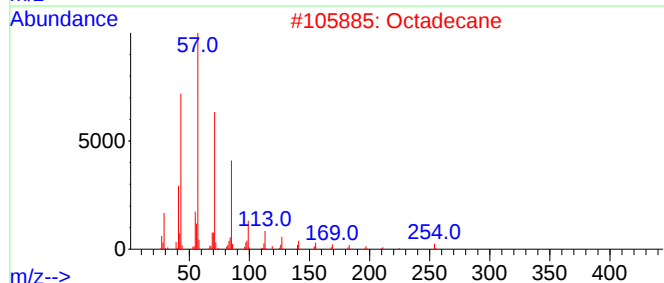
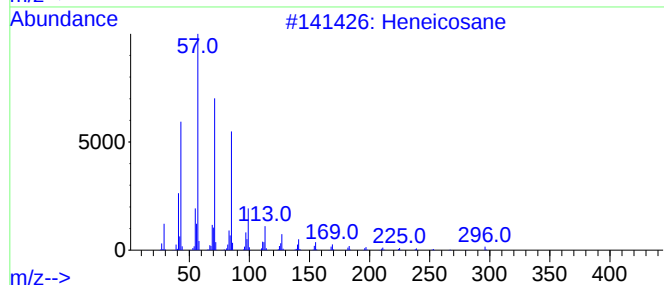
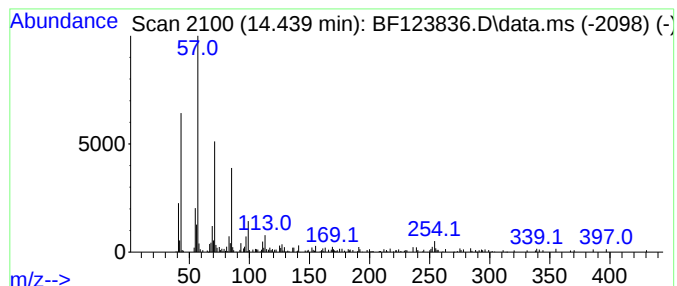
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.439	2.87 ng	186164	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	93
2			Octadecane	254	C18H38	000593-45-3	90
3			Octacosane	394	C28H58	000630-02-4	83
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
5			Tetracosane	338	C24H50	000646-31-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123836.D
Acq On : 5 May 2021 19:42
Operator : JU/CG
Sample : M2279-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-18

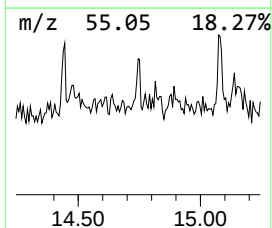
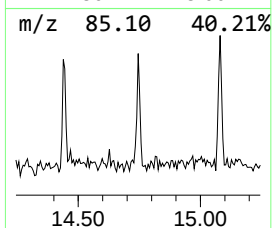
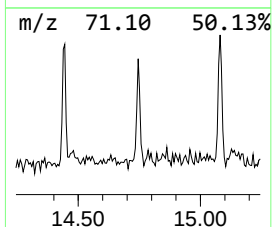
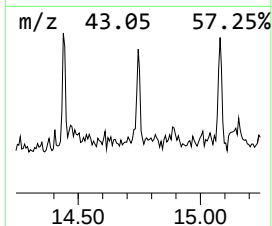
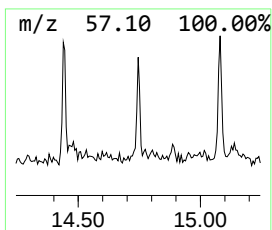
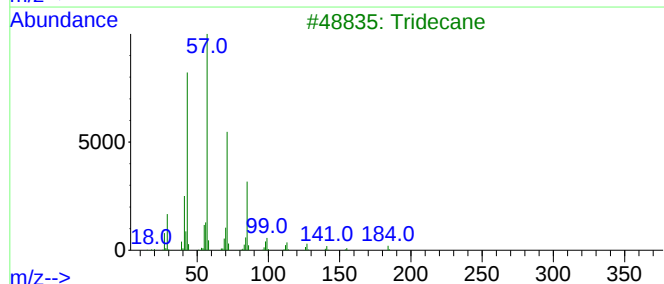
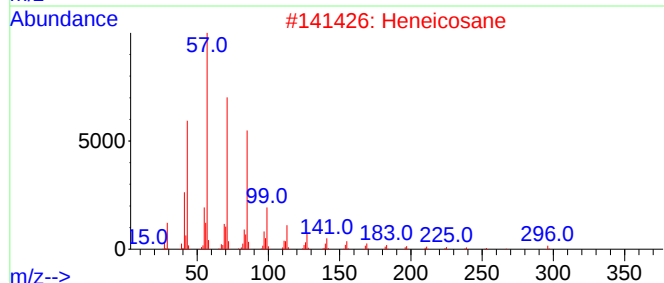
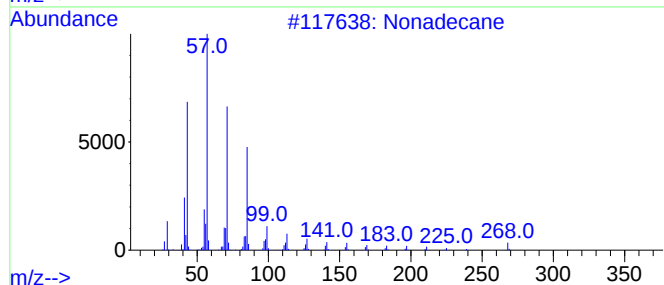
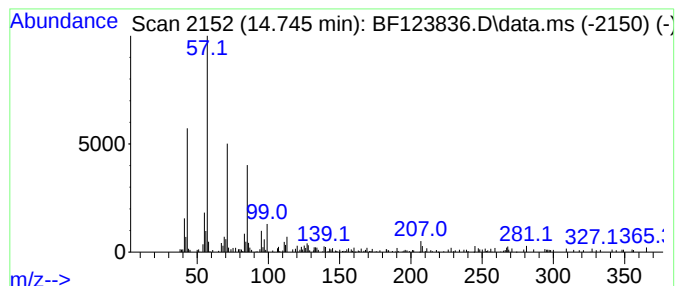
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	3.05 ng	131958	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	90
2			Heneicosane	296	C21H44	000629-94-7	89
3			Tridecane	184	C13H28	000629-50-5	74
4			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	74
5			Octadecane	254	C18H38	000593-45-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123836.D
Acq On : 5 May 2021 19:42
Operator : JU/CG
Sample : M2279-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

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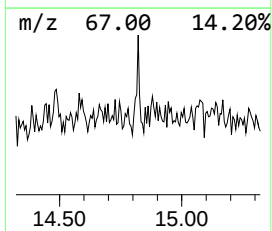
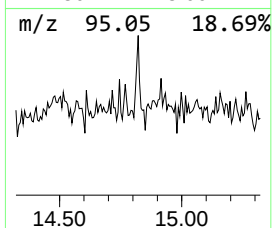
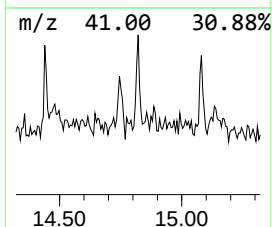
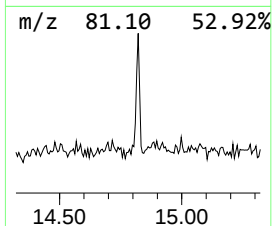
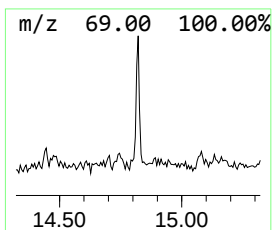
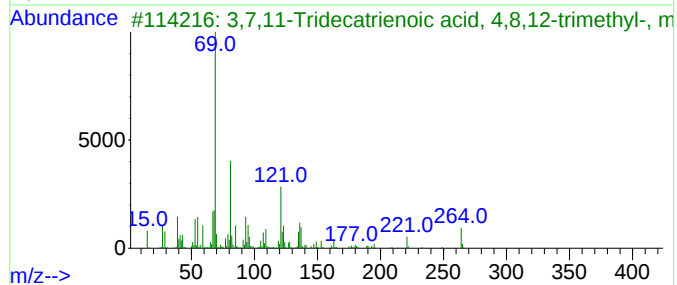
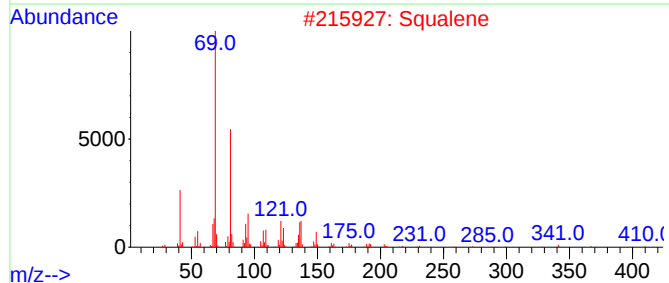
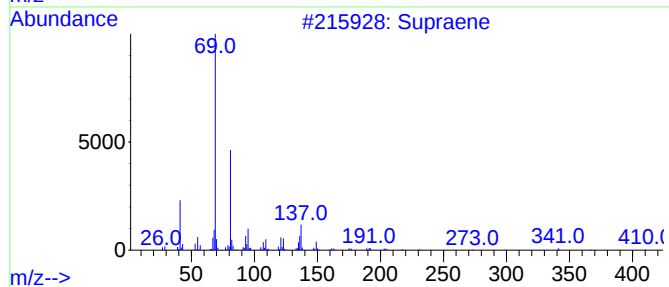
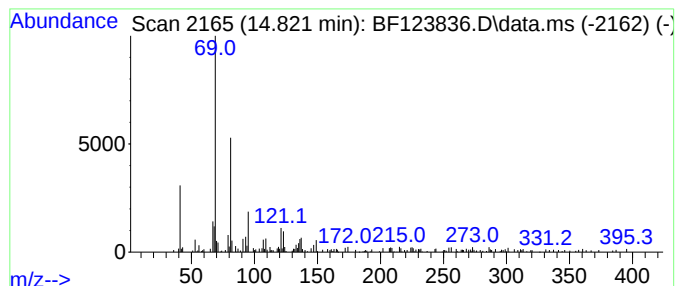
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	3.14 ng	135883	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			Squalene	410	C30H50	000111-02-4	80
3			3,7,11-Tridecatricienoic acid, 4,8...	264	C17H28O2	036237-70-4	64
4			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
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Acq On : 5 May 2021 19:42
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Sample : M2279-07
Misc :
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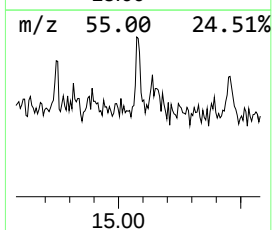
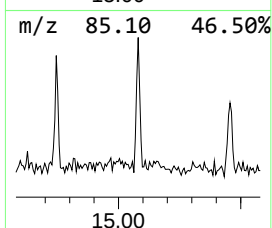
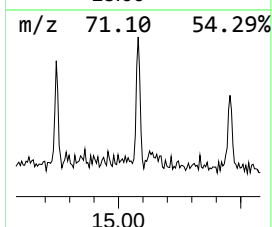
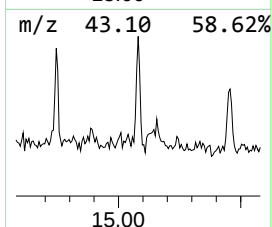
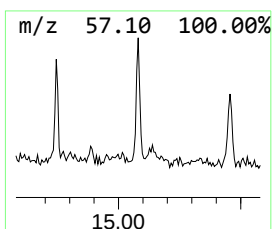
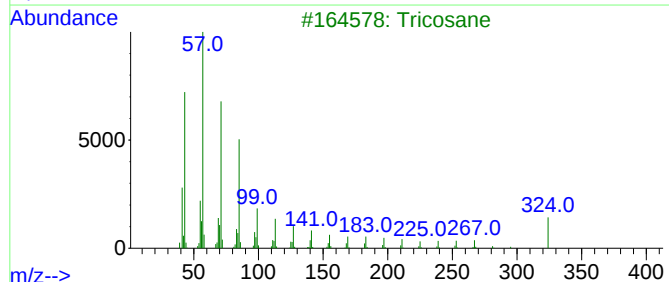
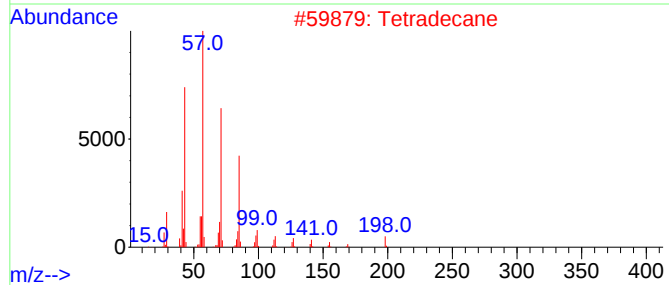
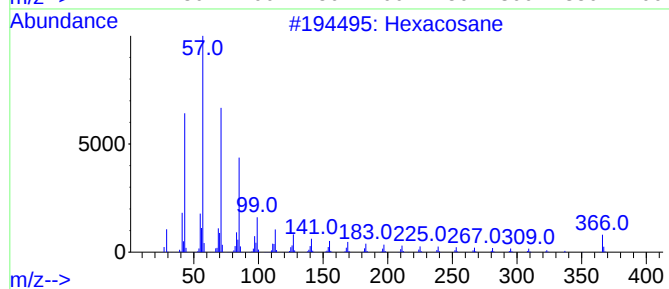
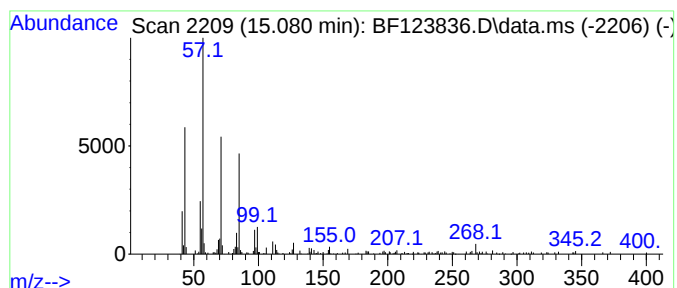
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.080	4.14 ng	178811	Perylene-d12	15.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	74
2	Tetradecane	198	C14H30	000629-59-4	72
3	Tricosane	324	C23H48	000638-67-5	72
4	Octacosane	394	C28H58	000630-02-4	64
5	Heptacosane	380	C27H56	000593-49-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123836.D
Acq On : 5 May 2021 19:42
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Sample : M2279-07
Misc :
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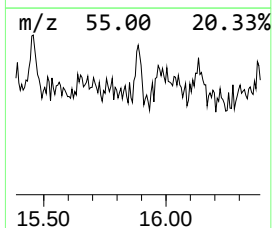
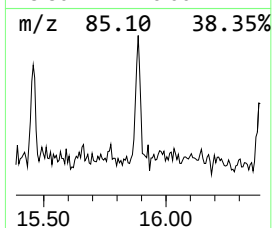
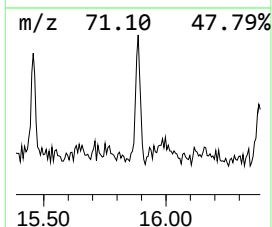
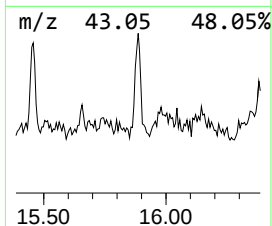
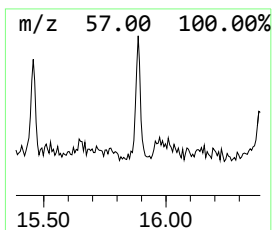
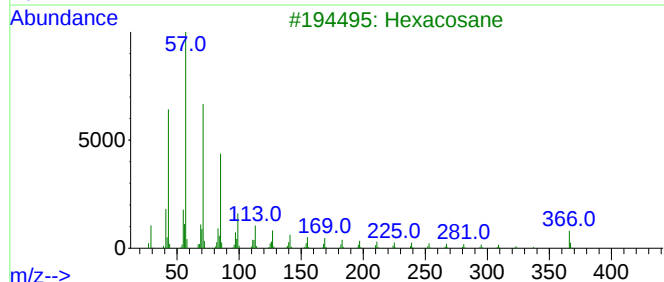
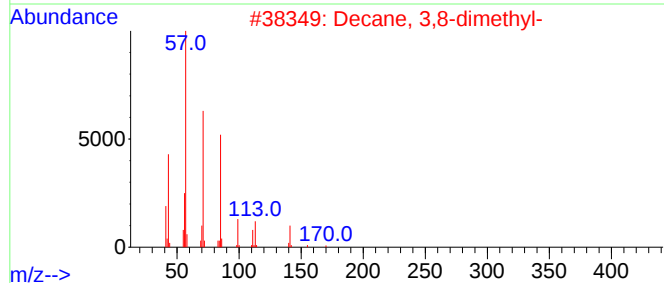
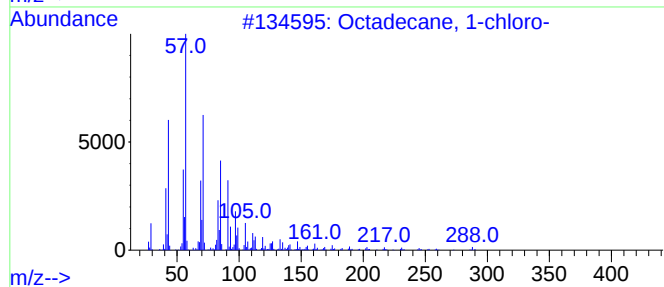
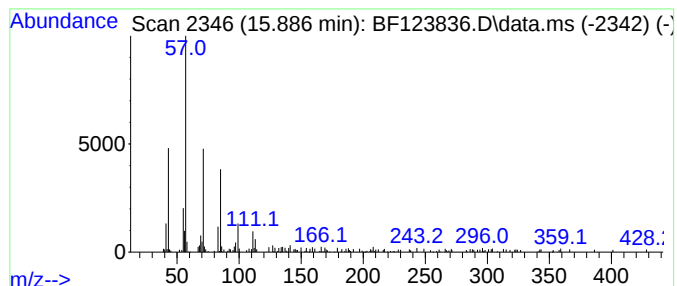
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane, 1-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.886	4.11 ng	177880	Perylene-d12	15.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	87
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	86
3	Hexacosane	366	C26H54	000630-01-3	80
4	Triacontane	422	C30H62	000638-68-6	72
5	Heneicosane	296	C21H44	000629-94-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123836.D
Acq On : 5 May 2021 19:42
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Sample : M2279-07
Misc :
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Instrument :
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ClientSampled :
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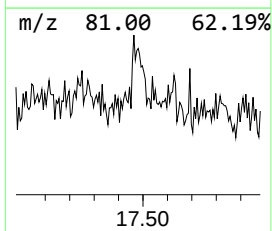
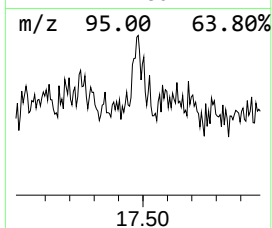
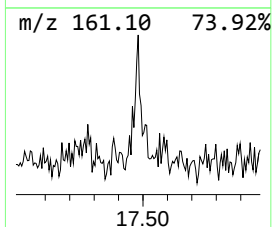
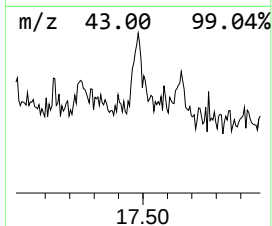
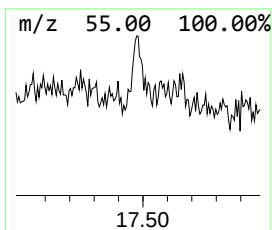
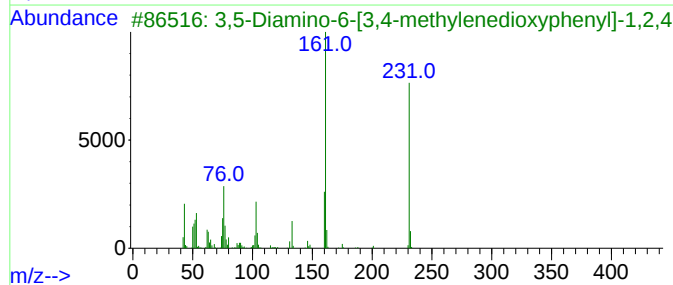
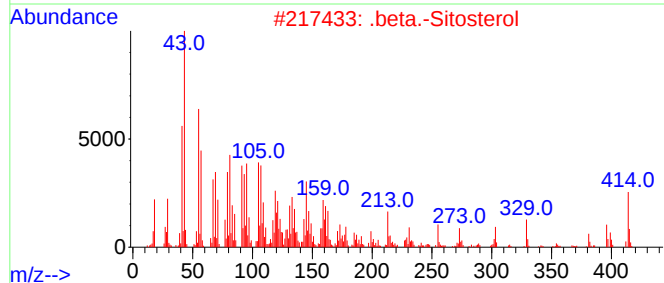
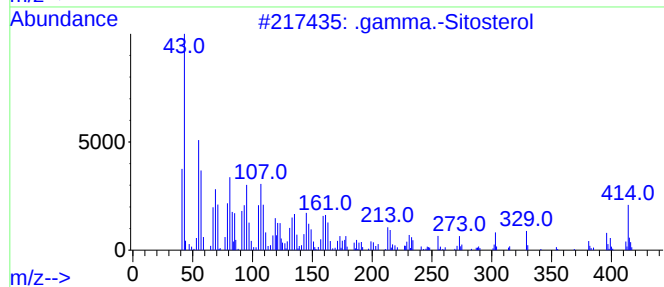
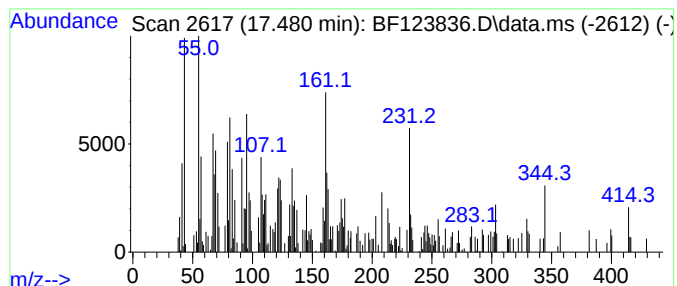
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.480 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.480	8.48 ng	366783	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	gamma.-	Sitosterol	414	C29H50O	000083-47-6	45
2	.	beta.-	Sitosterol	414	C29H50O	000083-46-5	44
3	3,5-	Diamino-6-[3,4-methylenedioxyphenyl]-	231	C10H9N5O2	058848-65-0	25	
4	1H-Benzimidazol-2-amine, 1-ethyl-	161	C9H11N3	001622-58-8	22		
5	Cholestan-3-one, 4,4-dimethyl-, ...	414	C29H50O	002097-85-0	20		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123836.D
Acq On : 5 May 2021 19:42
Operator : JU/CG
Sample : M2279-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EME-18

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
Tridecane, 6-me...	10.745	2.0	ng	151074	4	11.322	1505940	20.0
n-Hexadecanoic ...	11.857	3.8	ng	286786	4	11.322	1505940	20.0
unknown12.404	12.404	2.7	ng	205871	4	11.322	1505940	20.0
Eicosane	13.145	2.1	ng	137922	5	13.963	1296680	20.0
Cyclohexadecane...	13.822	12.1	ng	781036	5	13.963	1296680	20.0
Heneicosane	14.439	2.9	ng	186164	5	13.963	1296680	20.0
Nonadecane	14.745	3.0	ng	131958	6	15.421	864857	20.0
Supraene	14.821	3.1	ng	135883	6	15.421	864857	20.0
Hexacosane	15.080	4.1	ng	178811	6	15.421	864857	20.0
Octadecane, 1-c...	15.886	4.1	ng	177880	6	15.421	864857	20.0
unknown17.480	17.480	8.5	ng	366783	6	15.421	864857	20.0