

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
 Data File : BF123619.D
 Acq On : 19 Apr 2021 13:19
 Operator : JU/CG
 Sample : M2070-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JGD-3150-D3550-A

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-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123619.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	15	rVB	2340427	3013089	16.09%	4.523%
2	5.110	502	514	517	rBV	8811127	18726580	100.00%	28.108%
3	5.493	575	579	591	rVB	4103529	3504619	18.71%	5.260%
4	6.498	746	750	762	rVB	6010145	5947612	31.76%	8.927%
5	6.863	808	812	815	rBV	1972081	1484852	7.93%	2.229%
6	7.428	902	908	911	rBV	5041186	5189927	27.71%	7.790%
7	8.145	1026	1030	1033	rBV	2231944	1913667	10.22%	2.872%
8	9.228	1209	1214	1217	rBV	8136555	7049952	37.65%	10.582%
9	9.616	1277	1280	1283	rBV	316509	241485	1.29%	0.362%
10	9.904	1325	1329	1333	rVB	2331483	1975375	10.55%	2.965%
11	10.422	1406	1417	1421	rBV	230581	476684	2.55%	0.715%
12	10.627	1444	1452	1454	rBV4	265296	630027	3.36%	0.946%
13	10.692	1459	1463	1473	rVB	2232300	2087945	11.15%	3.134%
14	11.398	1579	1583	1585	rBV	2184203	2000511	10.68%	3.003%
15	11.922	1666	1672	1676	rBV3	263477	340216	1.82%	0.511%
16	12.121	1702	1706	1716	rVB4	112901	260133	1.39%	0.390%
17	12.863	1829	1832	1843	rVB3	207790	516780	2.76%	0.776%
18	12.986	1849	1853	1856	rBV	6403871	5734970	30.62%	8.608%
19	13.774	1980	1987	1996	rBV2	234926	558002	2.98%	0.838%
20	13.921	2005	2012	2021	rBV5	216437	538138	2.87%	0.808%
21	14.039	2028	2032	2035	rBV	1882434	1584136	8.46%	2.378%
22	14.421	2092	2097	2102	rBV	285536	498417	2.66%	0.748%
23	15.015	2193	2198	2205	rBV	251025	429158	2.29%	0.644%
24	15.521	2279	2284	2288	rBV2	1080033	1378214	7.36%	2.069%
25	15.674	2304	2310	2317	rVB3	163513	350586	1.87%	0.526%
26	16.439	2435	2440	2446	rBV4	99901	192541	1.03%	0.289%

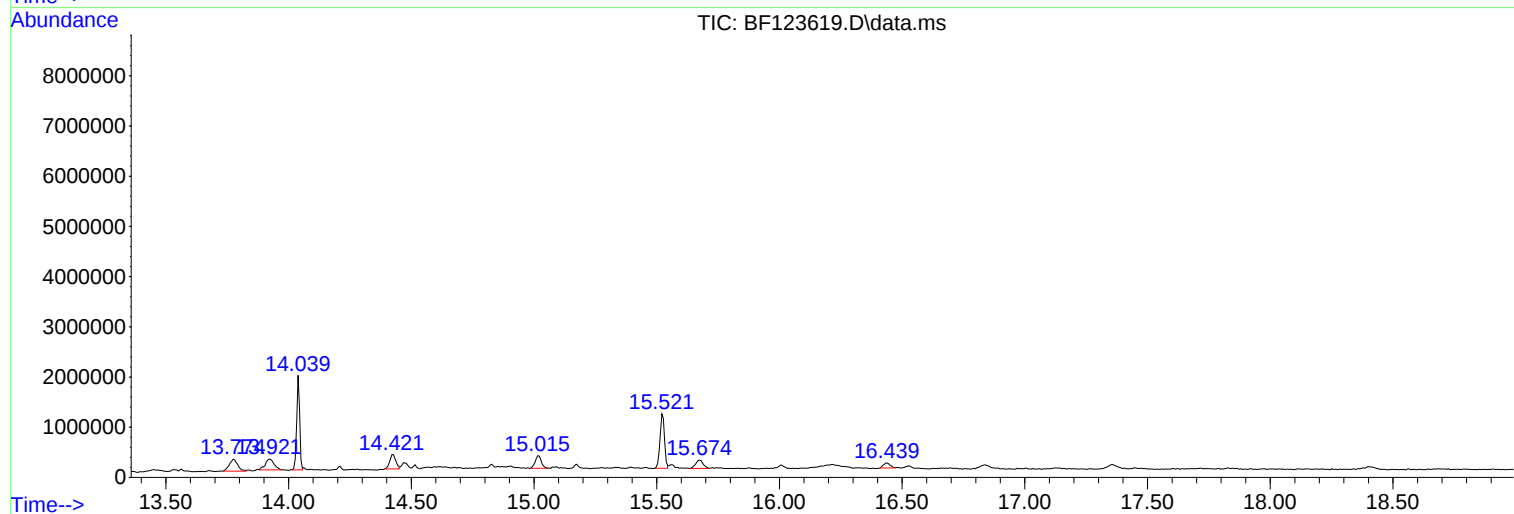
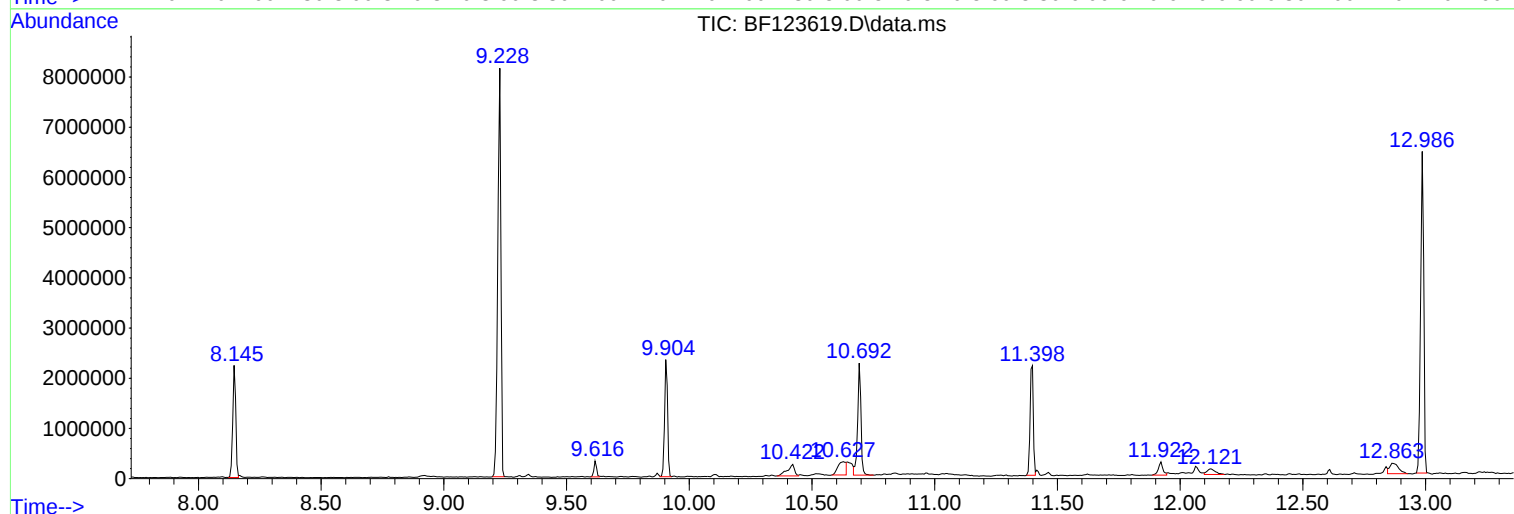
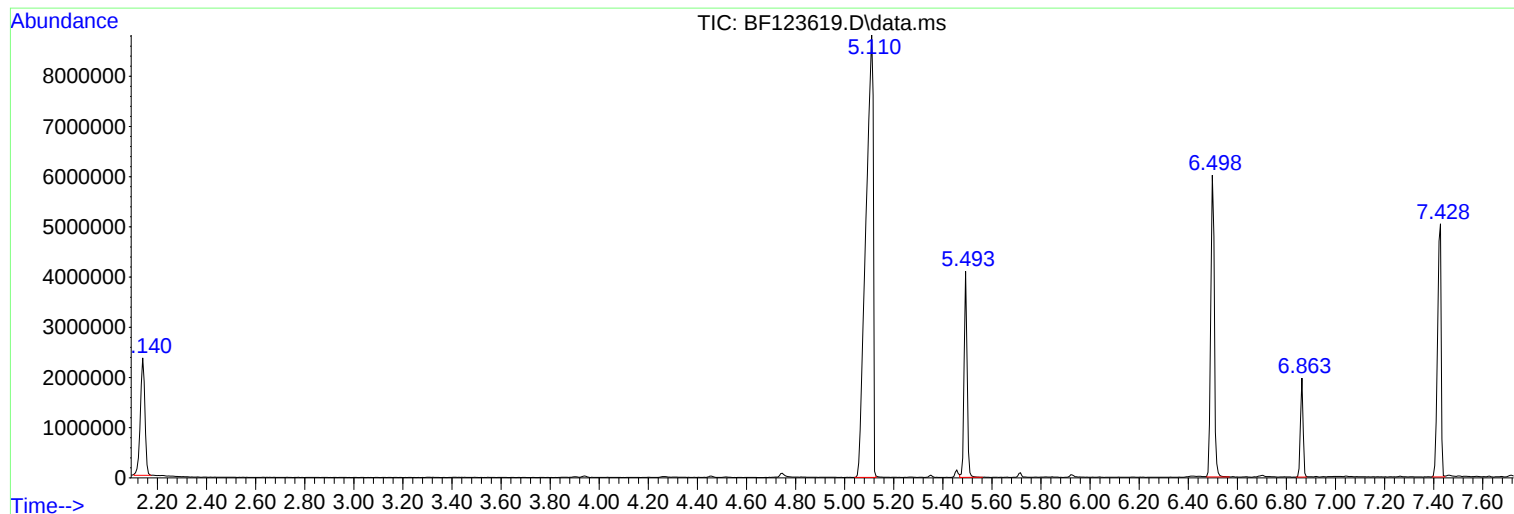
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ClientSampleId :
JGD-3150-D3550-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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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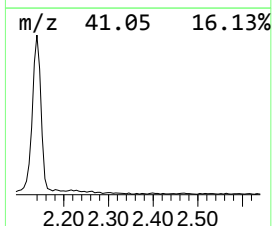
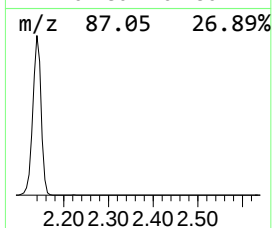
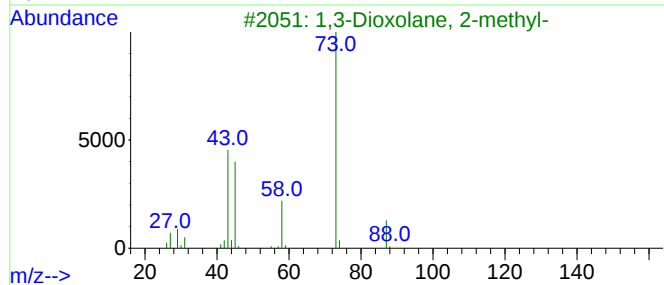
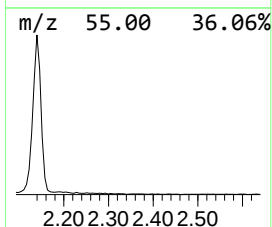
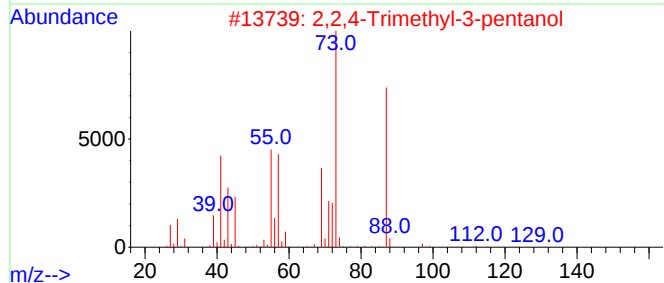
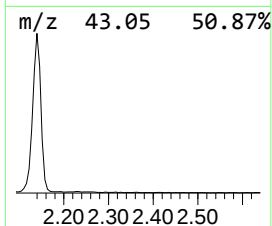
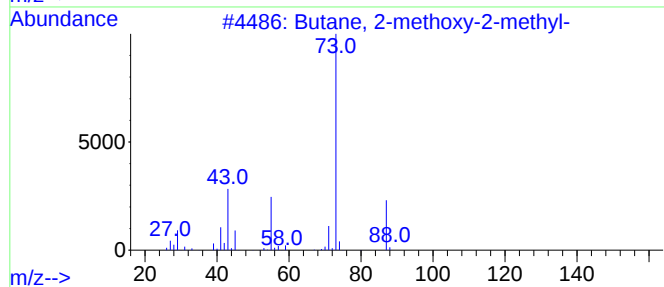
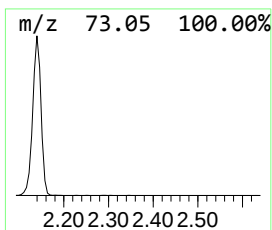
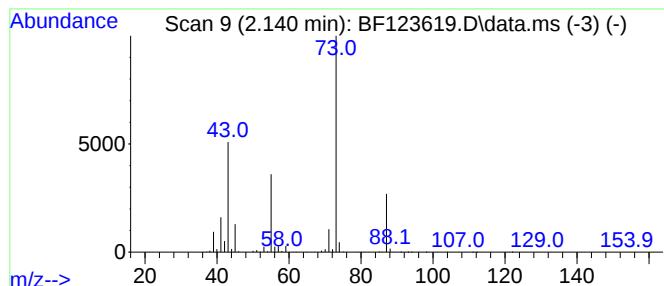
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	40.58 ng	3013090	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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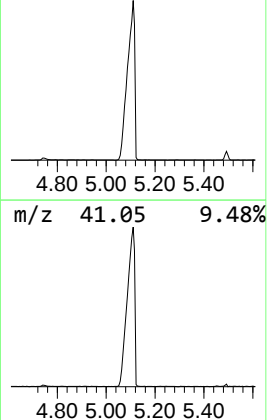
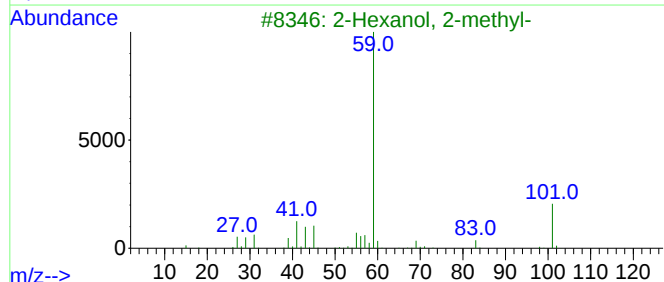
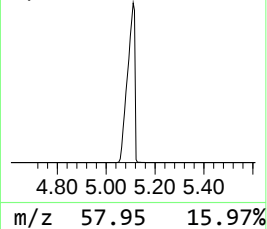
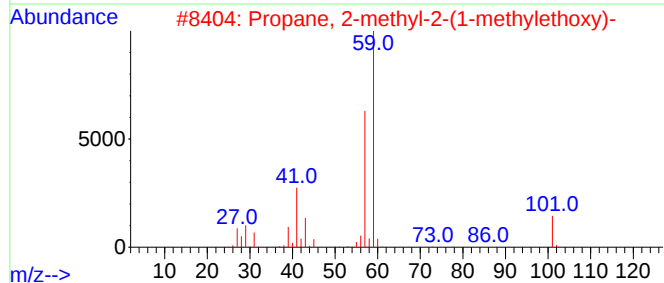
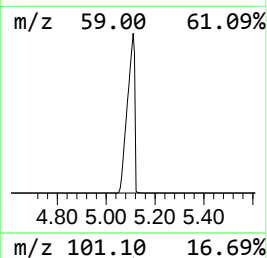
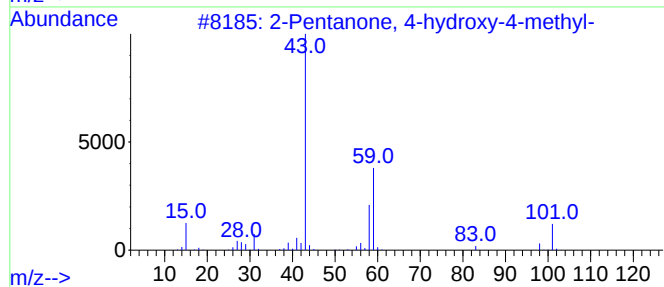
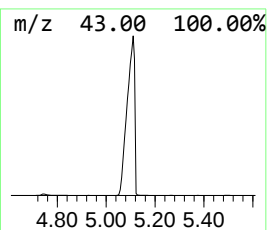
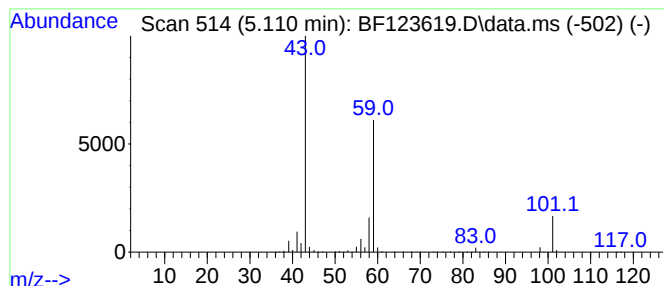
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	252.24 ng	18726600	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		



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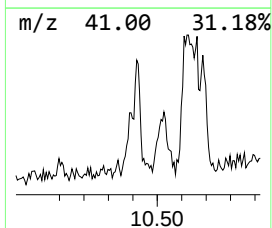
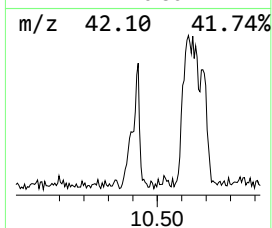
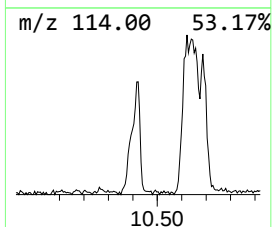
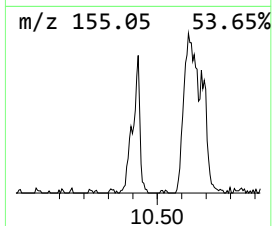
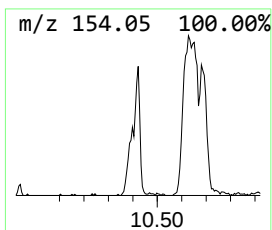
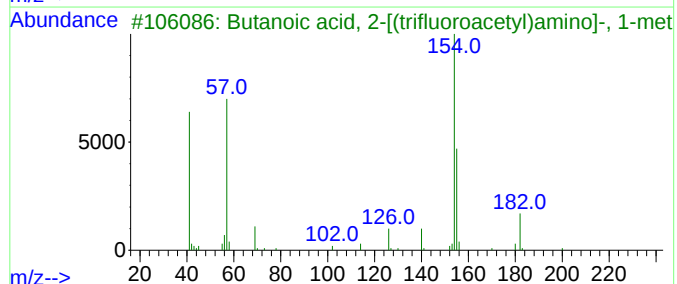
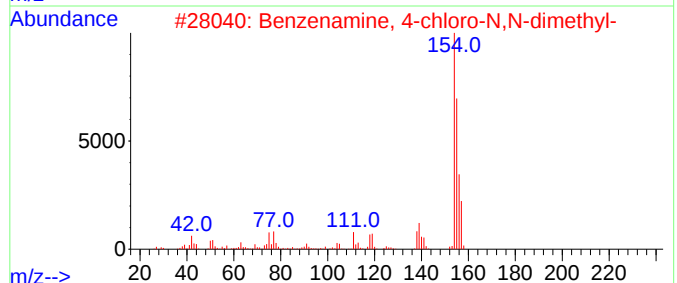
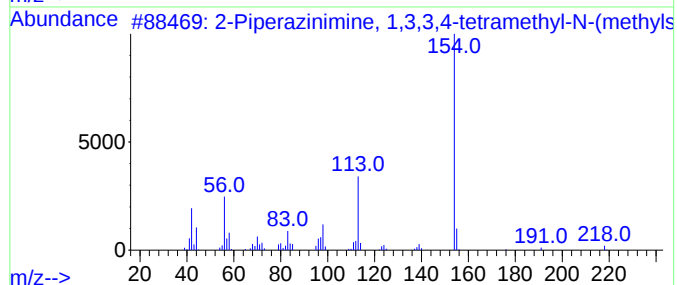
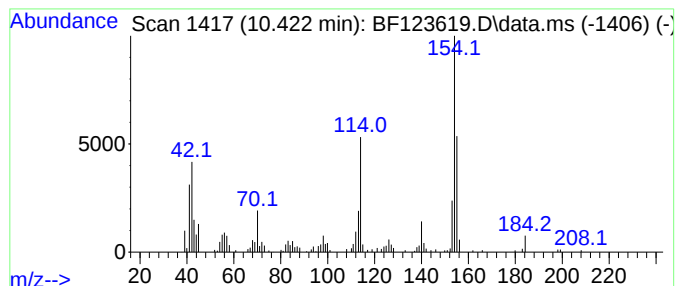
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.42 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.422	4.83 ng	476684	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperazinimine, 1,3,3,4-tetram...	233	C9H19N3O2S	1000221-39-0	38		
2	Benzenamine, 4-chloro-N,N-dimethyl-	155	C8H10ClN	000698-69-1	35		
3	Butanoic acid, 2-[(trifluoroacet...	255	C10H16F3NO3	054986-68-4	32		
4	Biphenyl	154	C12H10	000092-52-4	27		
5	Acetonitrile, (3-methyl-4-oxo-2-...	154	C6H6N2OS	056196-65-7	25		



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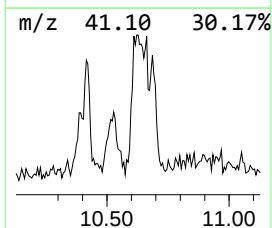
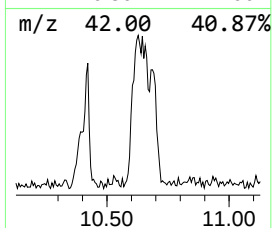
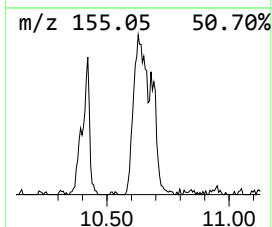
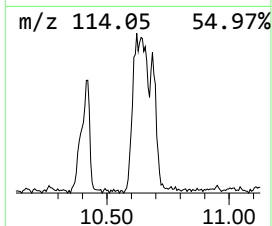
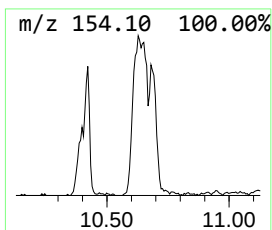
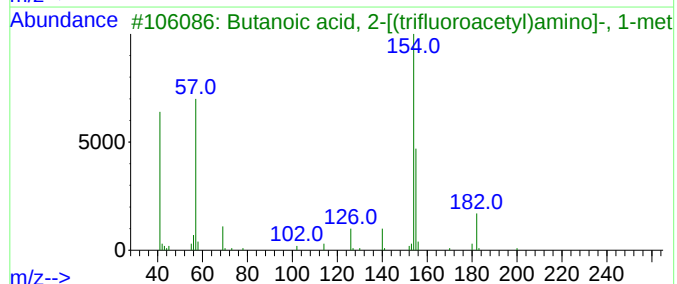
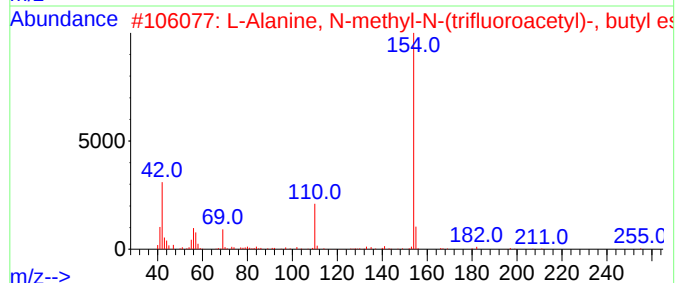
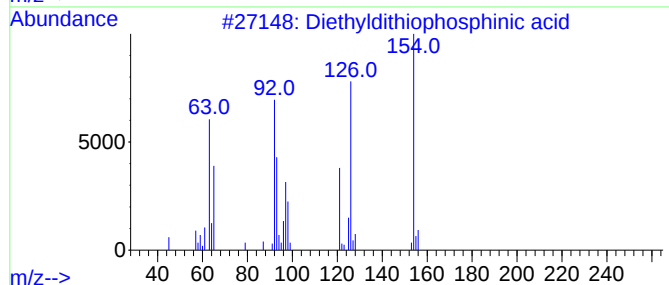
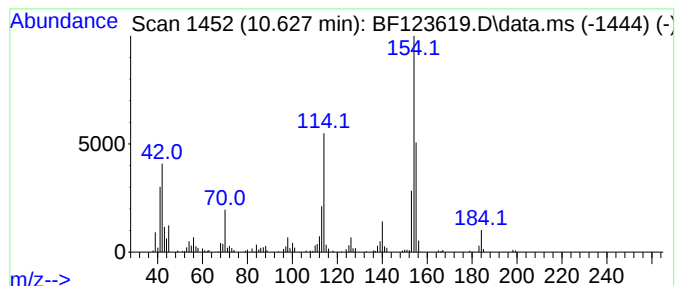
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Peak Number 4 unknown10.62 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	6.38 ng	630027	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyldithiophosphinic acid	154	C4H11PS2	000866-54-6	30
2			L-Alanine, N-methyl-N-(trifluoro...	255	C10H16F3NO3	034815-08-2	27
3			Butanoic acid, 2-[(trifluoroacet...	255	C10H16F3NO3	054986-68-4	23
4			Benzene, 1-methoxy-3-(methylthio)-	154	C8H10OS	002388-74-1	14
5			Sebacic acid, 2,6-dimethoxypheny...	520	C31H52O6	1000354-76-0	14



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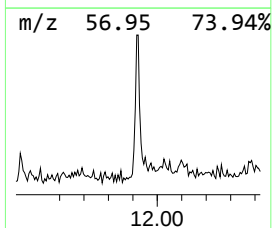
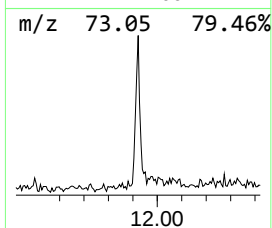
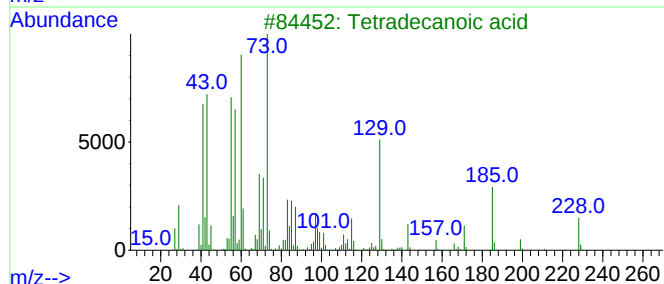
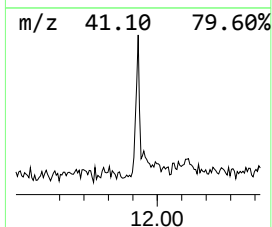
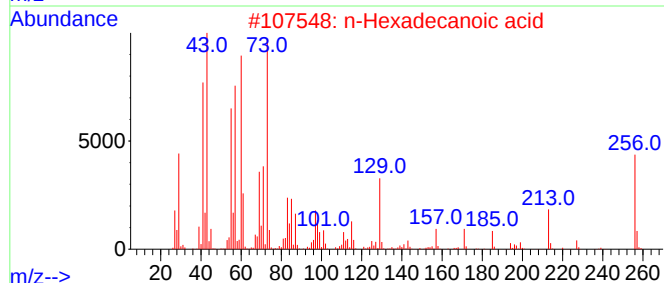
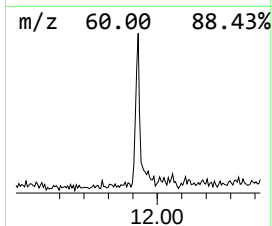
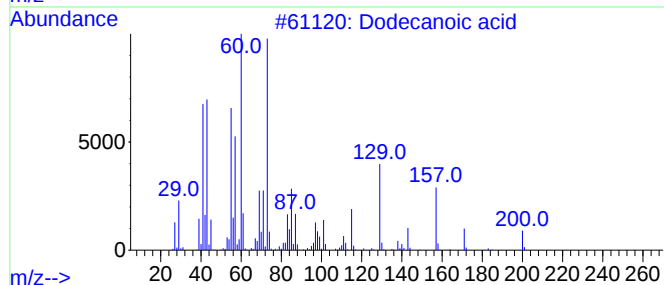
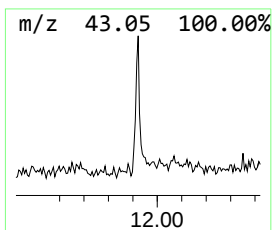
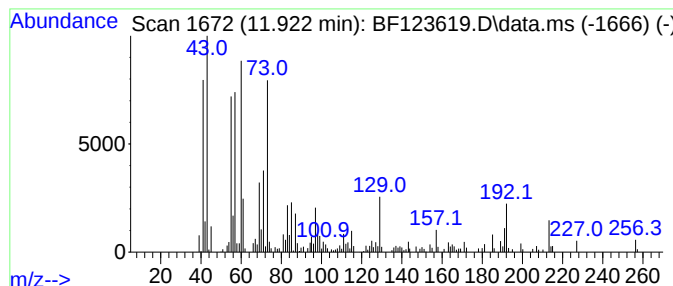
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Dodecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.40 ng	340216	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	86
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4			Tridecanoic acid	214	C13H26O2	000638-53-9	58
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



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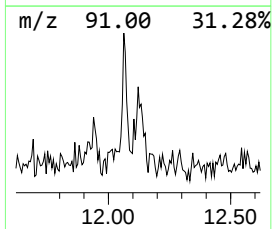
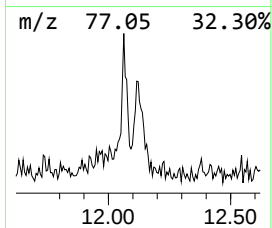
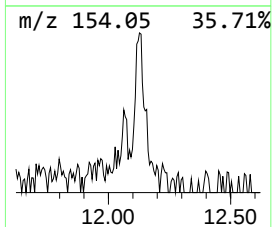
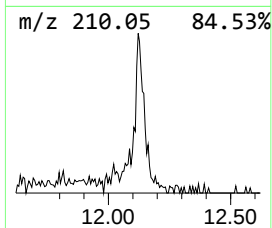
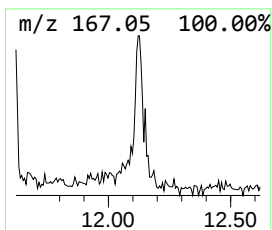
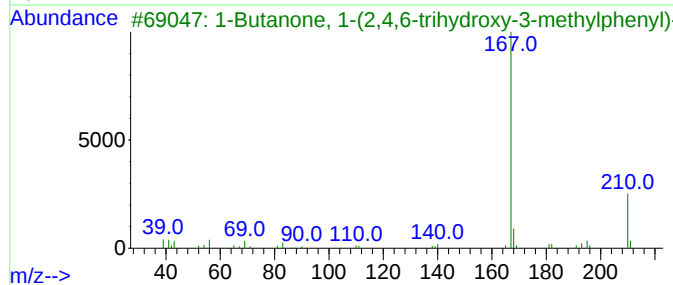
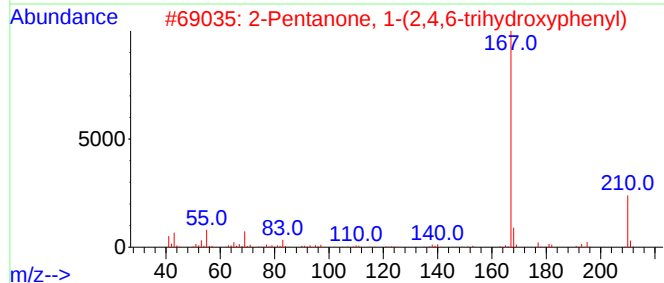
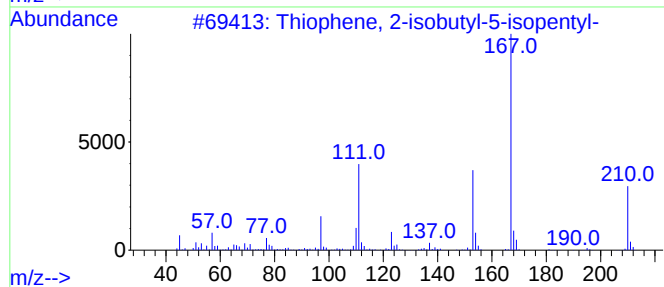
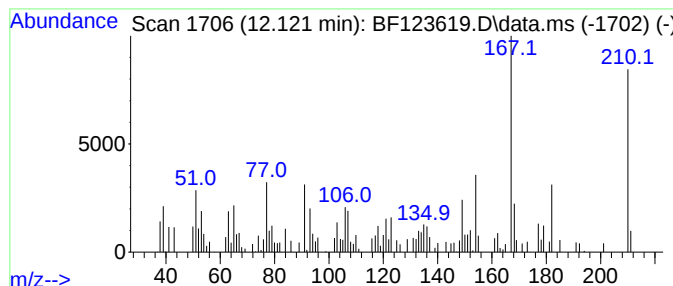
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.12 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.121	2.60 ng	260133	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2-isobutyl-5-isopentyl-	210	C13H22S	004806-10-4	49
2			2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	49
3			1-Butanone, 1-(2,4,6-trihydroxy-...	210	C11H14O4	001509-06-4	47
4			2-Methoxythiobenzamide	167	C8H9NOS	042590-97-6	27
5			Benzene, 1,1'-ethyldienebis-	182	C14H14	000612-00-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123619.D
Acq On : 19 Apr 2021 13:19
Operator : JU/CG
Sample : M2070-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JGD-3150-D3550-A

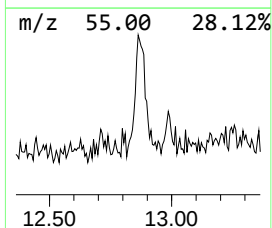
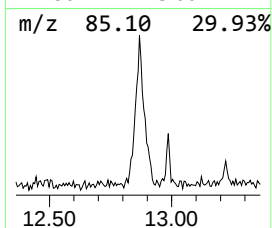
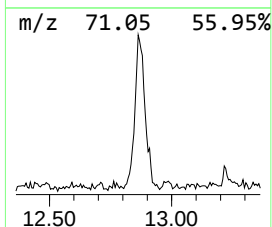
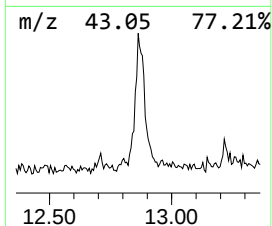
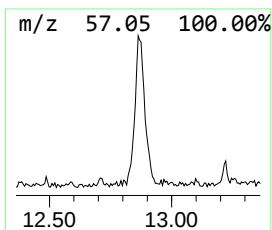
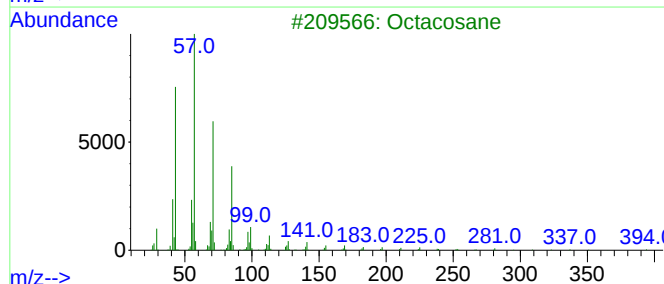
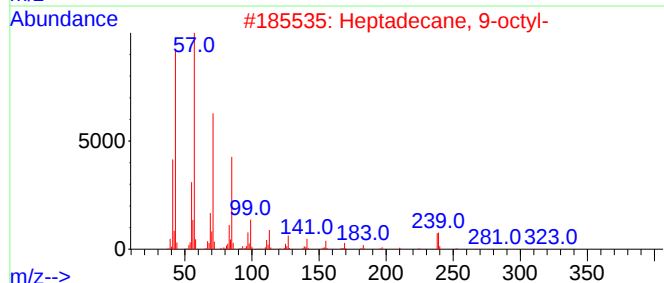
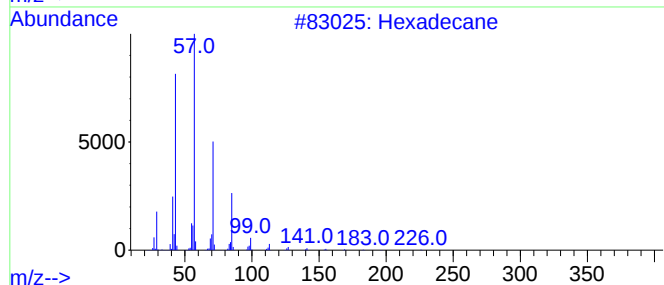
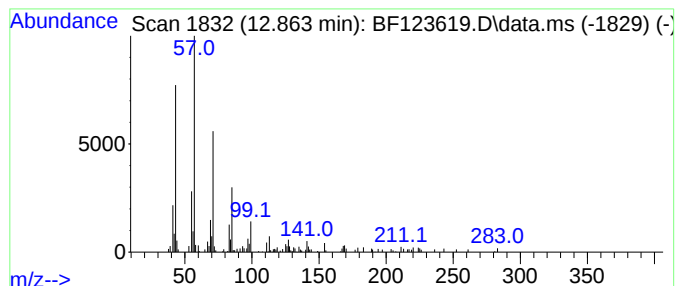
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.863	6.52 ng	516780	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	87
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	83
5			Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123619.D
Acq On : 19 Apr 2021 13:19
Operator : JU/CG
Sample : M2070-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
JGD-3150-D3550-A

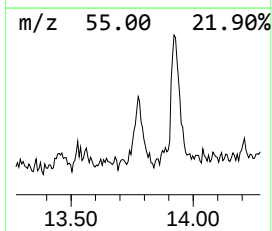
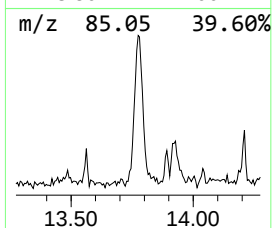
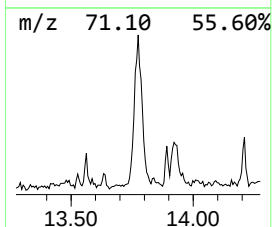
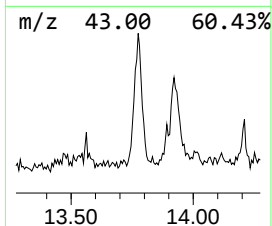
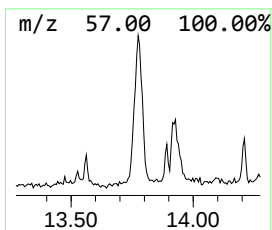
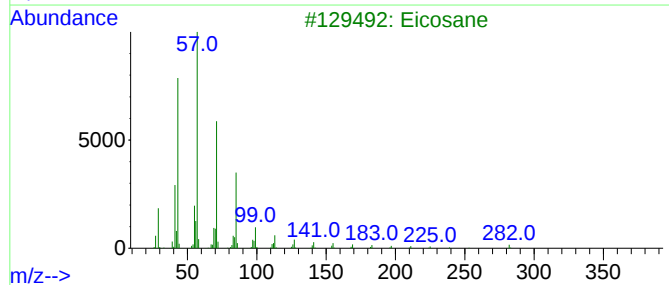
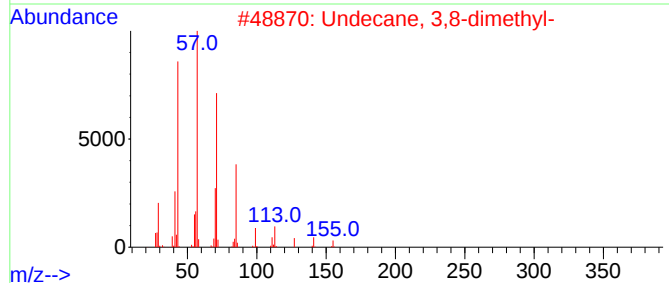
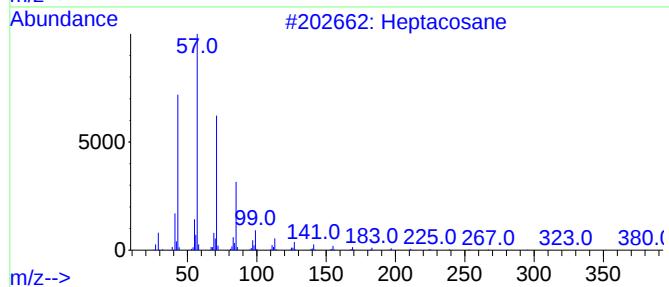
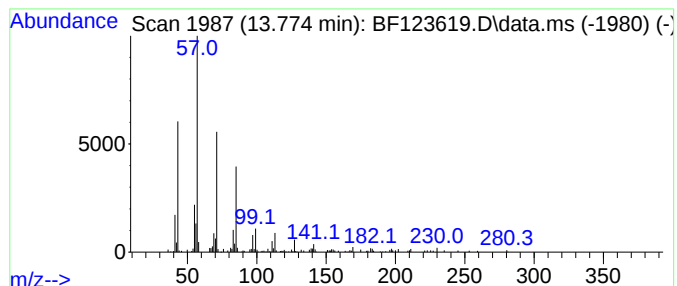
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	7.04 ng	558002	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	90
3			Eicosane	282	C20H42	000112-95-8	87
4			Octadecane	254	C18H38	000593-45-3	86
5			Tetradecane	198	C14H30	000629-59-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123619.D
Acq On : 19 Apr 2021 13:19
Operator : JU/CG
Sample : M2070-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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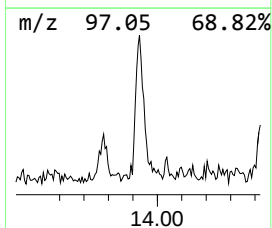
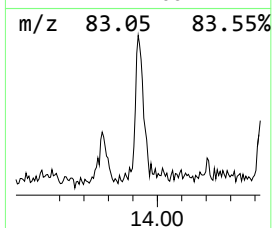
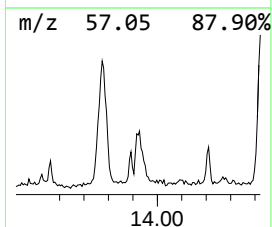
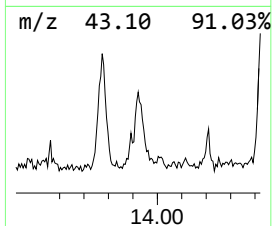
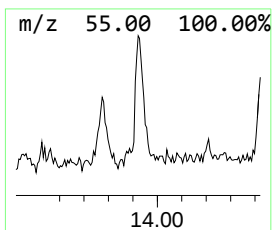
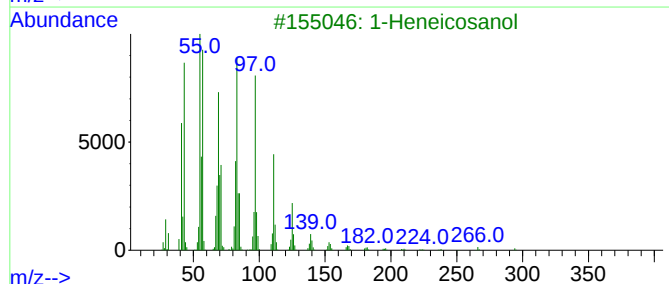
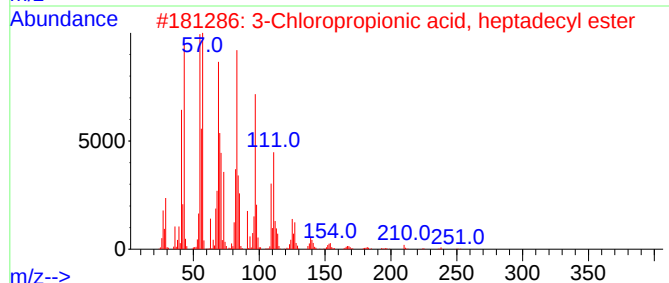
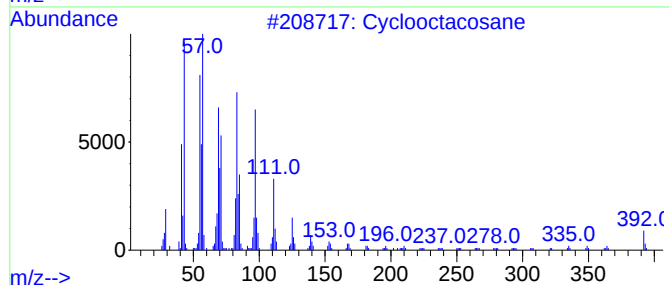
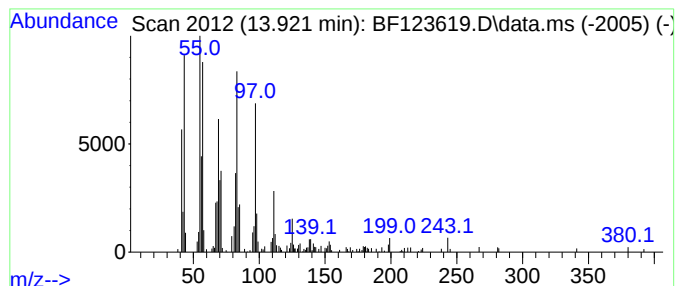
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclooctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	6.79 ng	538138	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctacosane	392	C28H56	000297-24-5	93
2			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3			1-Heneicosanol	312	C21H44O	015594-90-8	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123619.D
Acq On : 19 Apr 2021 13:19
Operator : JU/CG
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Misc :
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Instrument :
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ClientSampleId :
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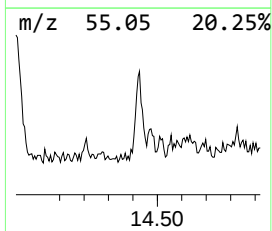
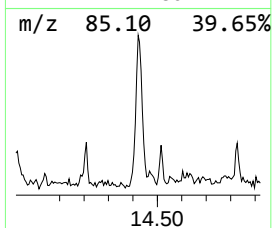
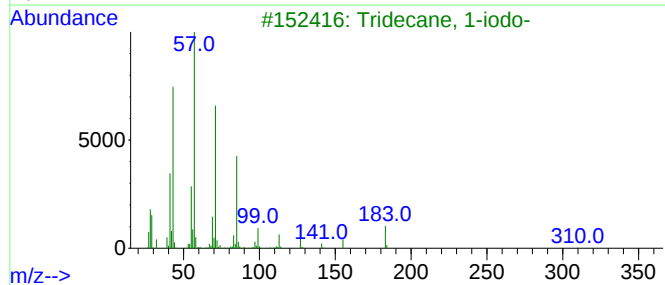
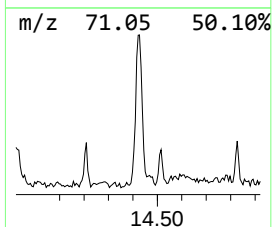
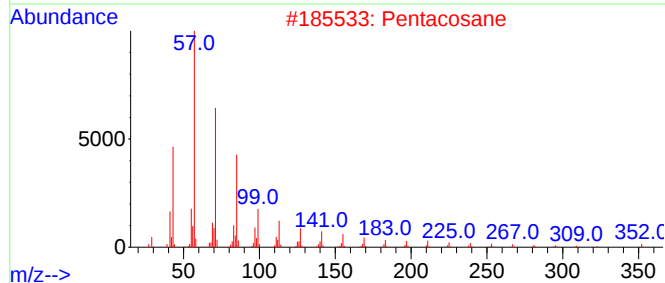
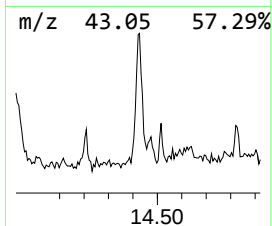
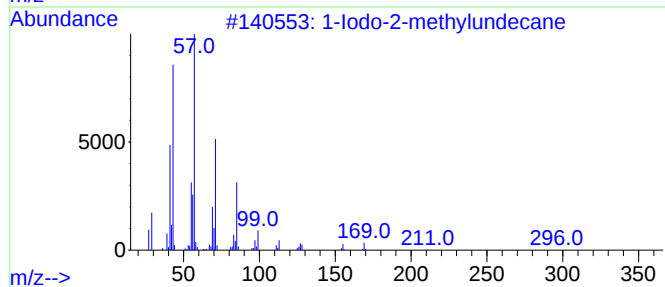
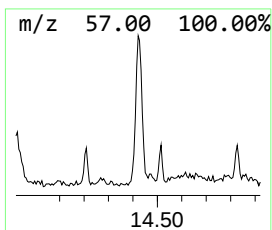
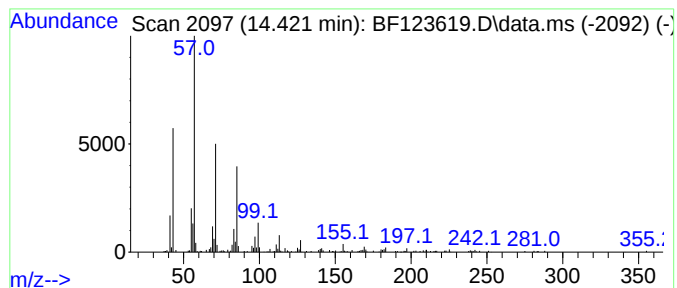
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Iodo-2-methylundecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.421	6.29 ng	498417	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90
2			Pentacosane	352	C25H52	000629-99-2	90
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
4			Octacosane	394	C28H58	000630-02-4	86
5			2-Bromo dodecane	248	C12H25Br	013187-99-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123619.D
Acq On : 19 Apr 2021 13:19
Operator : JU/CG
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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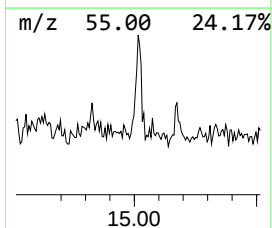
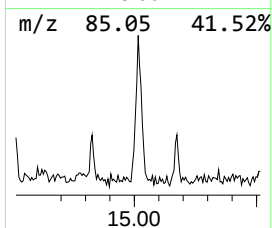
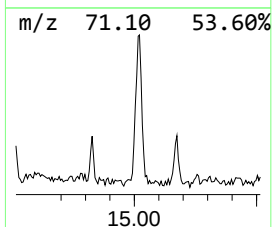
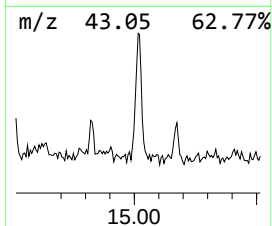
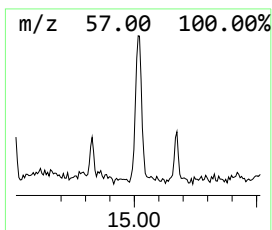
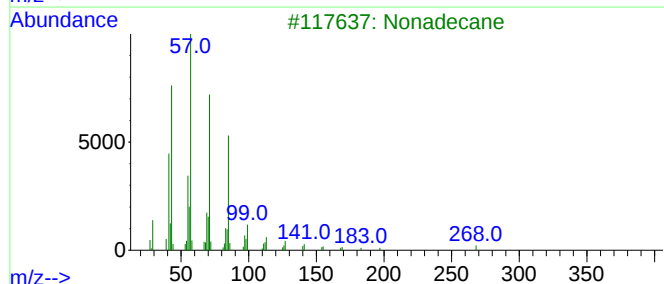
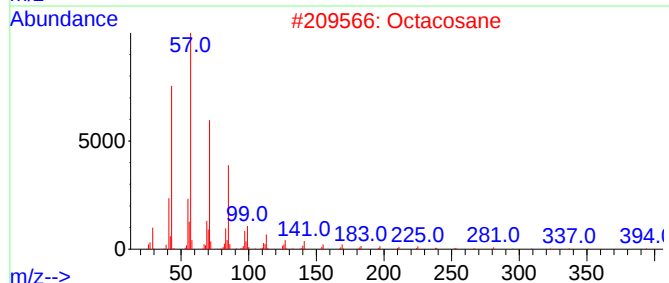
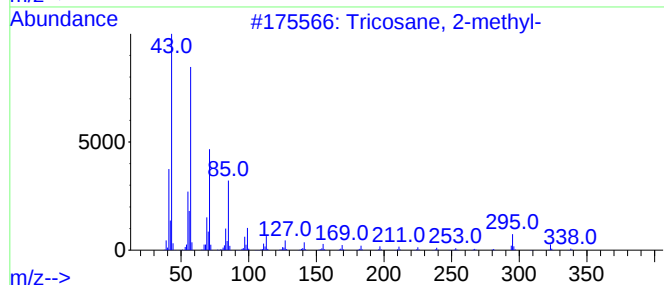
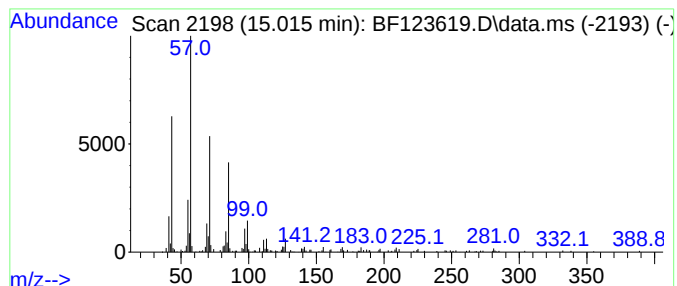
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tricosane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.015	6.23 ng	429158	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane, 2-methyl-	338	C24H50	001928-30-9	93
2			Octacosane	394	C28H58	000630-02-4	90
3			Nonadecane	268	C19H40	000629-92-5	87
4			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	86
5			Docosane, 2,21-dimethyl-	338	C24H50	077536-31-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123619.D
Acq On : 19 Apr 2021 13:19
Operator : JU/CG
Sample : M2070-01
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ClientSampleId :
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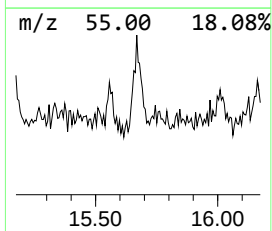
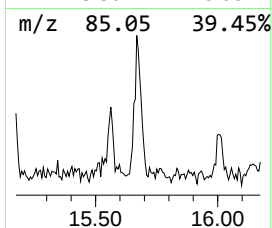
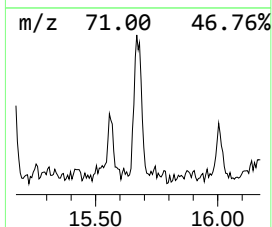
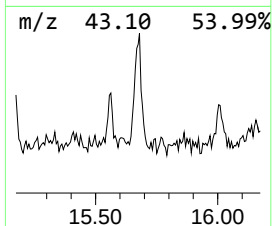
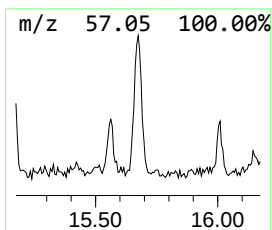
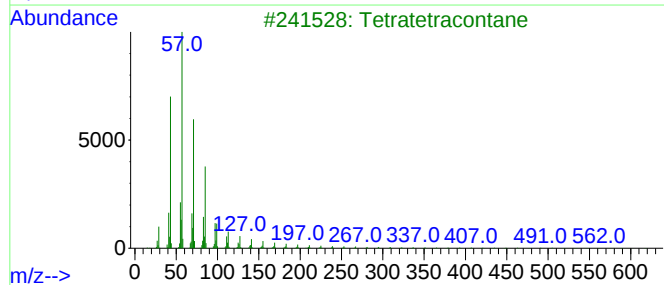
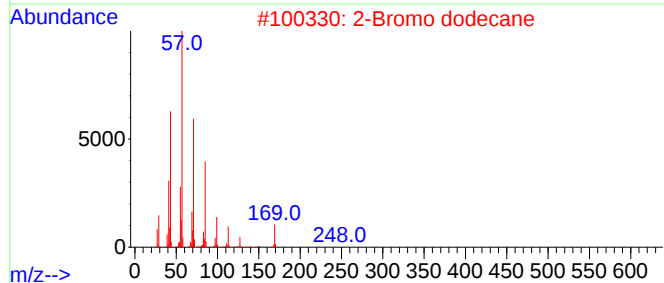
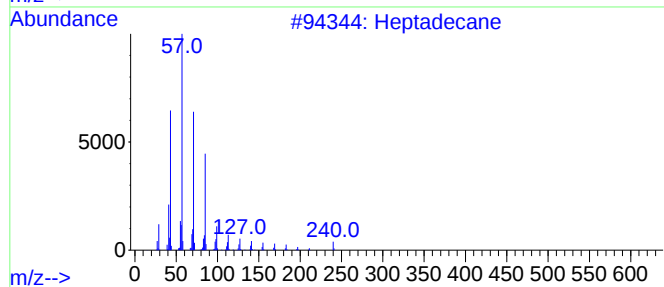
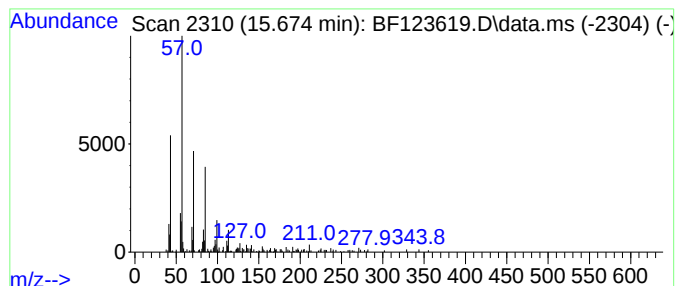
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.674	5.09 ng	350586	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	86
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	86
3			Tetratetracontane	619	C44H90	007098-22-8	86
4			Tetradecane	198	C14H30	000629-59-4	74
5			Octadecane	254	C18H38	000593-45-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
Data File : BF123619.D
Acq On : 19 Apr 2021 13:19
Operator : JU/CG
Sample : M2070-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JGD-3150-D3550-A

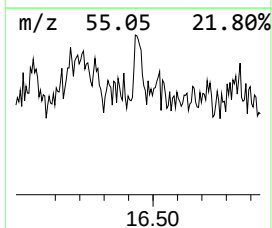
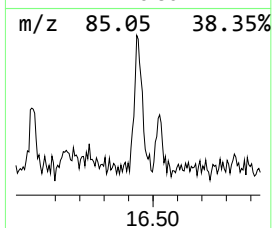
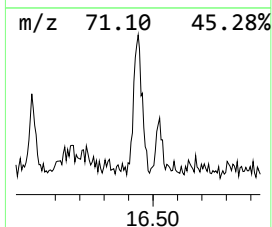
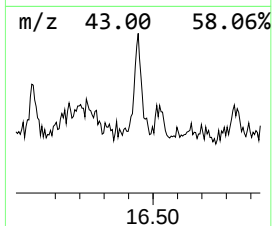
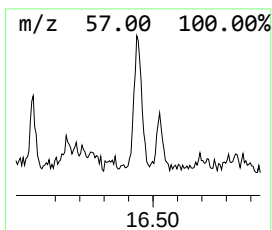
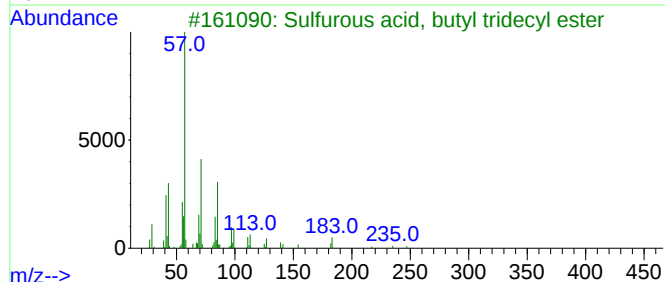
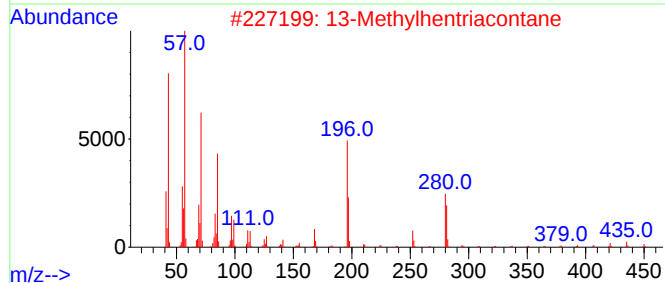
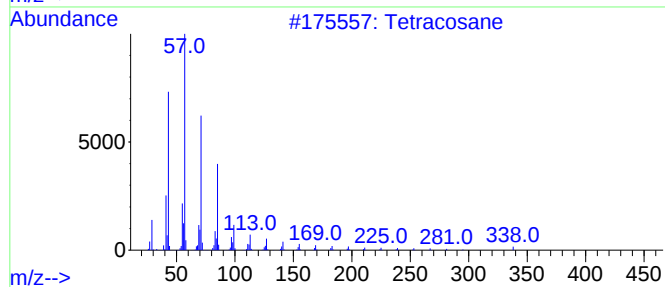
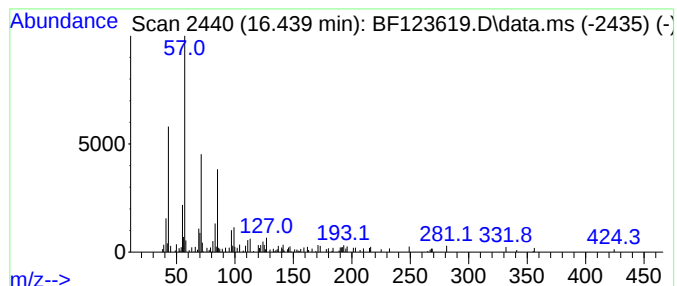
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.439	2.79 ng	192541	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	80
2			13-Methylhentriacontane	451	C32H66	1000131-19-4	78
3			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	78
4			Heptacosane	380	C27H56	000593-49-7	74
5			Nonadecane	268	C19H40	000629-92-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041921\
 Data File : BF123619.D
 Acq On : 19 Apr 2021 13:19
 Operator : JU/CG
 Sample : M2070-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JGD-3150-D3550-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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
Butane, 2-metho...	2.140	40.6	ng	3013090	1	6.863	1484850	20.0
2-Pentanone, 4-...	5.110	252.2	ng	18726600	1	6.863	1484850	20.0
unknown10.42	10.422	4.8	ng	476684	3	9.904	1975380	20.0
unknown10.62	10.628	6.4	ng	630027	3	9.904	1975380	20.0
Dodecanoic acid	11.922	3.4	ng	340216	4	11.398	2000510	20.0
unknown12.12	12.121	2.6	ng	260133	4	11.398	2000510	20.0
Hexadecane	12.863	6.5	ng	516780	5	14.039	1584140	20.0
Heptacosane	13.774	7.0	ng	558002	5	14.039	1584140	20.0
Cyclooctacosane	13.921	6.8	ng	538138	5	14.039	1584140	20.0
1-Iodo-2-methyl...	14.421	6.3	ng	498417	5	14.039	1584140	20.0
Tricosane, 2-me...	15.015	6.2	ng	429158	6	15.521	1378210	20.0
Heptadecane	15.674	5.1	ng	350586	6	15.521	1378210	20.0
Tetracosane	16.439	2.8	ng	192541	6	15.521	1378210	20.0