

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
 Data File : BF124175.D
 Acq On : 8 Jun 2021 12:09
 Operator : JU/CG
 Sample : M2613-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 18-B12(90-94)

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-BF060321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124175.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	13	rVB	572397	726387	49.40%	6.764%
2	5.493	575	579	582	rBV	1221146	1161640	79.00%	10.817%
3	6.504	746	751	754	rBV	1254382	1147278	78.02%	10.684%
4	6.857	808	811	814	rBV	262642	203735	13.86%	1.897%
5	7.422	902	907	910	rBV	839169	776502	52.81%	7.231%
6	8.045	1010	1013	1023	rBB2	19156	30761	2.09%	0.286%
7	8.140	1025	1029	1032	rBV	318163	259785	17.67%	2.419%
8	9.222	1208	1213	1216	rBV	1595146	1470416	100.00%	13.693%
9	9.898	1324	1328	1331	rBV	391752	315830	21.48%	2.941%
10	10.692	1458	1463	1466	rBV	1213329	1063538	72.33%	9.904%
11	11.386	1577	1581	1584	rBV	403337	327209	22.25%	3.047%
12	11.910	1666	1670	1673	rBV2	41465	43730	2.97%	0.407%
13	12.616	1774	1790	1800	rBV3	74287	227522	15.47%	2.119%
14	12.974	1846	1851	1854	rBV	1703296	1419632	96.55%	13.220%
15	13.610	1951	1959	1968	rBV4	79901	198298	13.49%	1.847%
16	13.892	2002	2007	2014	rBV8	23872	56937	3.87%	0.530%
17	14.027	2027	2030	2034	rVB	297289	247778	16.85%	2.307%
18	14.316	2071	2079	2083	rBV2	118425	199122	13.54%	1.854%
19	14.357	2083	2086	2091	rVB6	21854	30477	2.07%	0.284%
20	14.651	2132	2136	2138	rBV4	15184	18763	1.28%	0.175%
21	14.898	2170	2178	2184	rBV3	96061	186370	12.67%	1.736%
22	15.510	2276	2282	2286	rBV	174616	243500	16.56%	2.268%
23	15.557	2287	2290	2298	rVB4	55950	121707	8.28%	1.133%
24	16.321	2411	2420	2429	rBV4	40029	116780	7.94%	1.087%
25	16.715	2483	2487	2493	rVB8	14911	29944	2.04%	0.279%
26	17.210	2564	2571	2579	rVB5	28260	78593	5.34%	0.732%
27	18.280	2745	2753	2756	rBV9	14348	36452	2.48%	0.339%

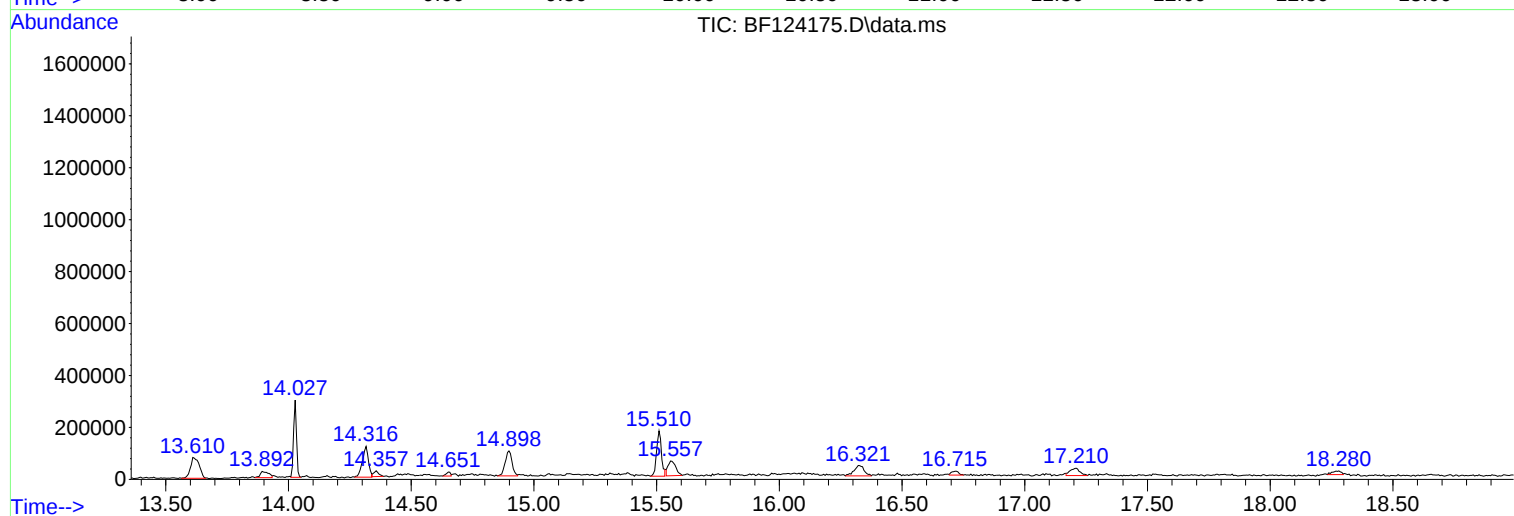
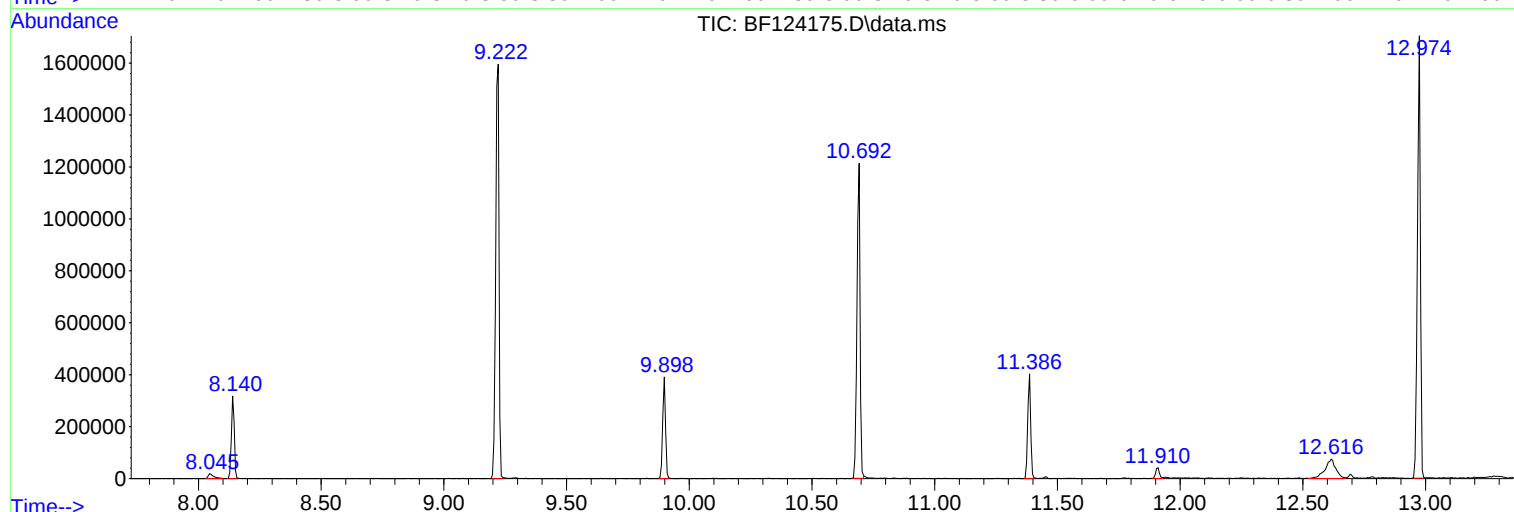
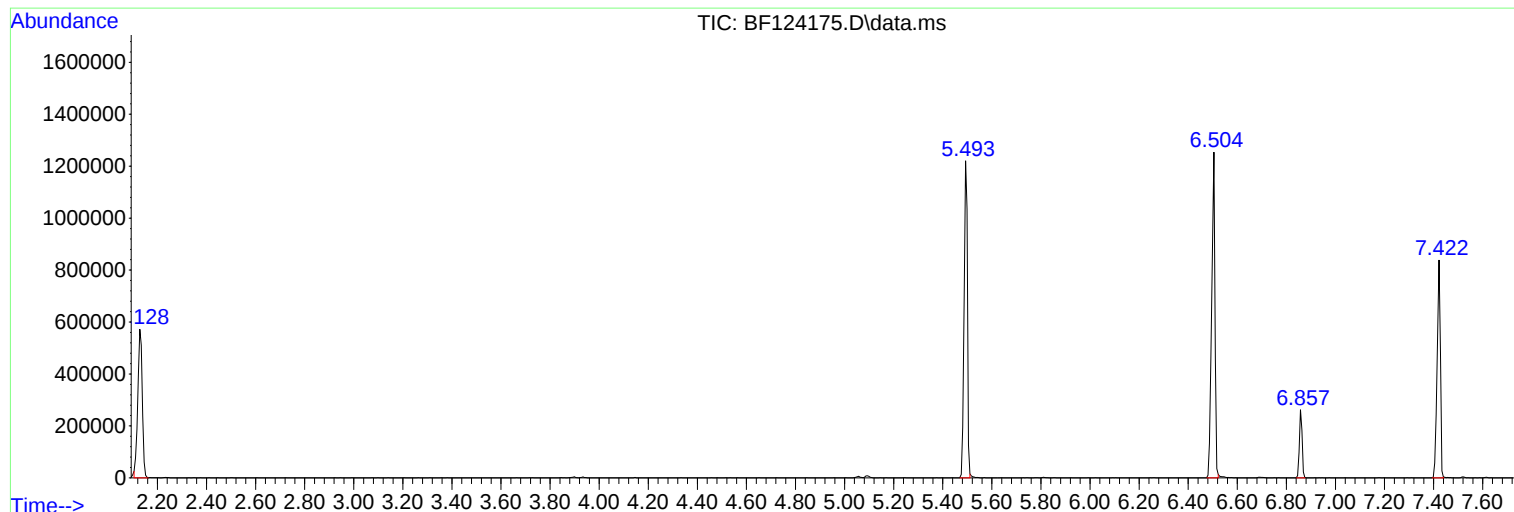
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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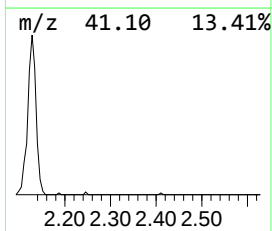
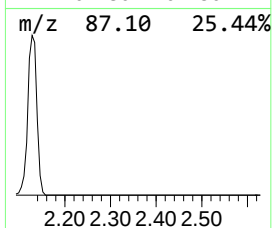
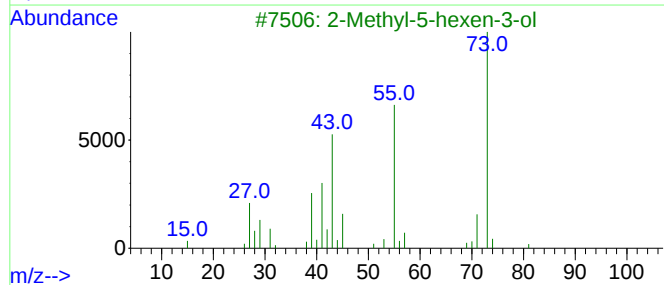
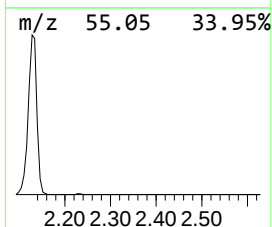
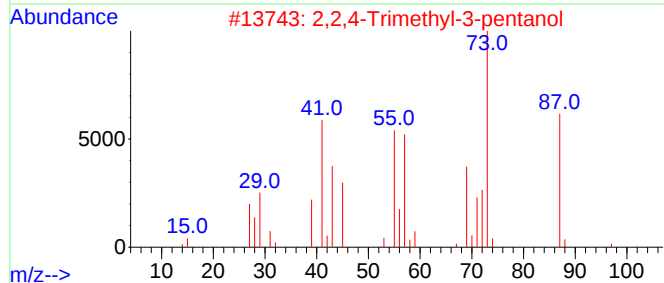
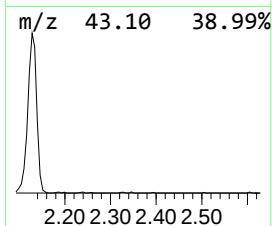
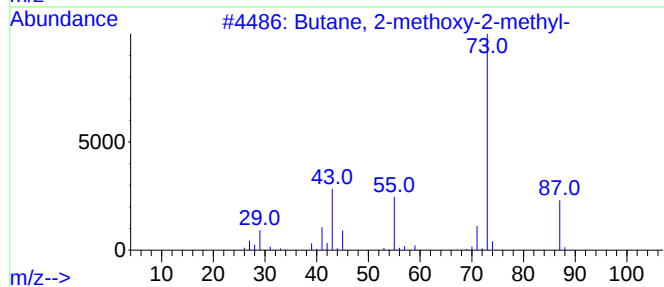
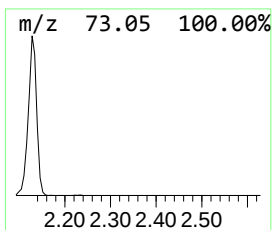
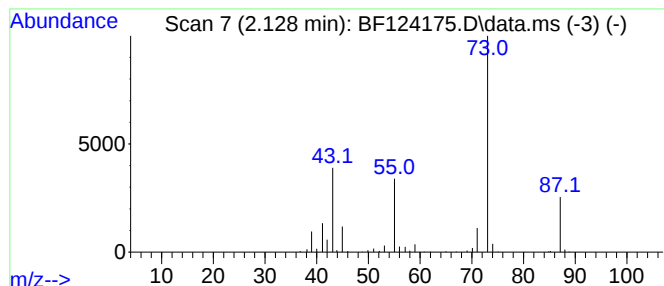
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	71.31 ng	726387	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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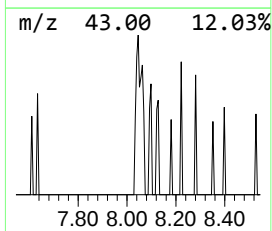
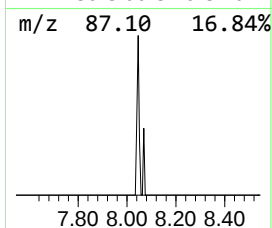
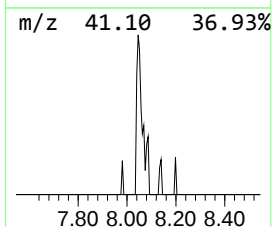
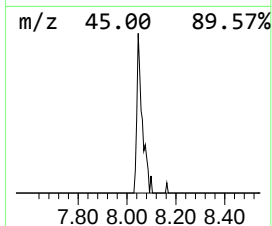
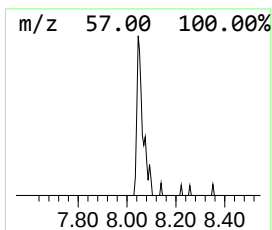
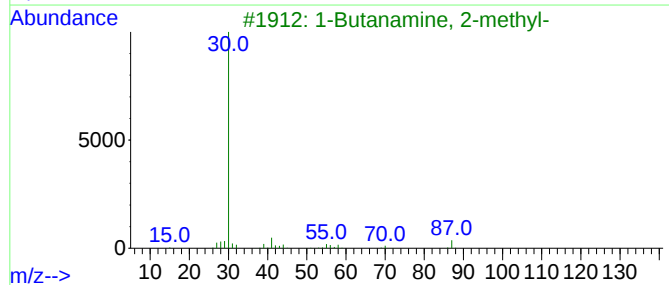
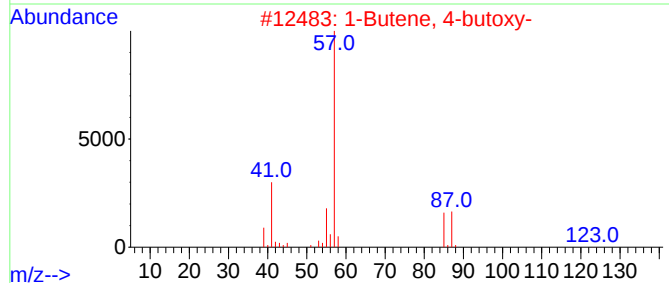
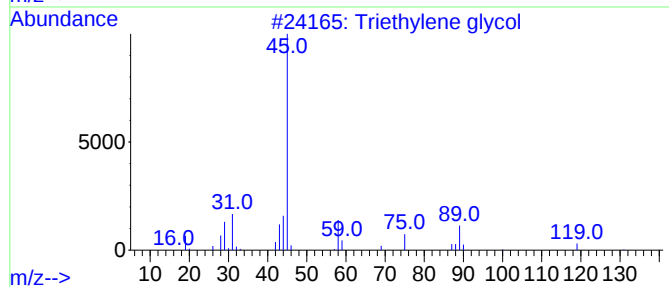
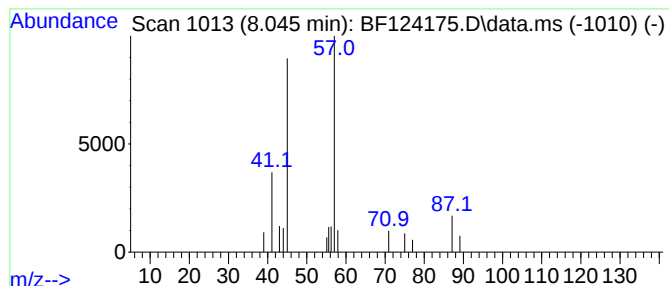
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown8.045 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.045	2.37 ng	30761	Naphthalene-d8	8.140

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triethylene glycol	150	C6H14O4	000112-27-6	33
2			1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	10
3			1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	9
4			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9



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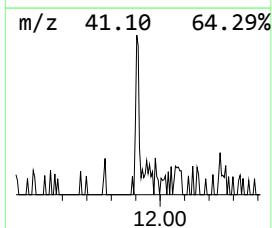
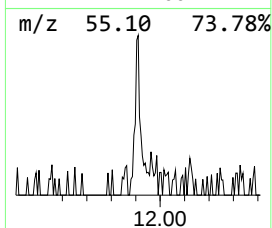
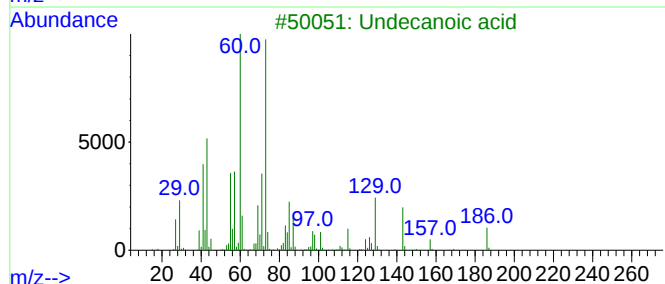
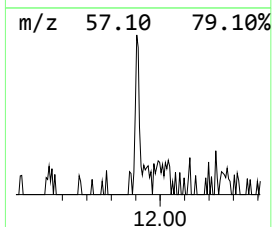
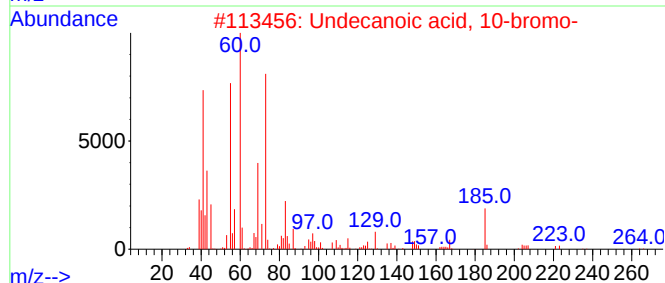
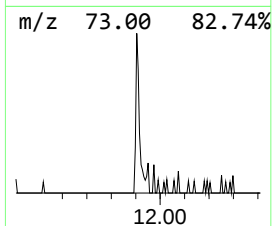
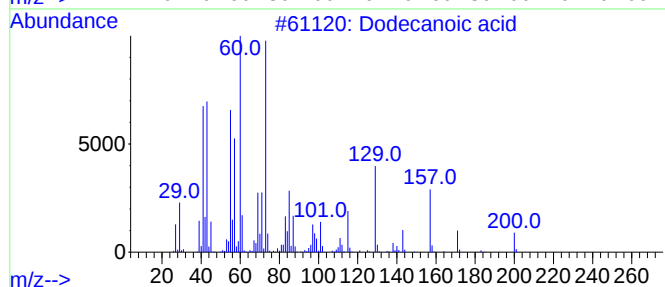
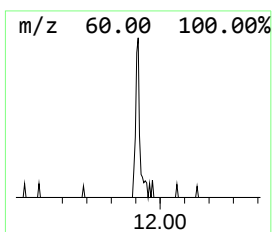
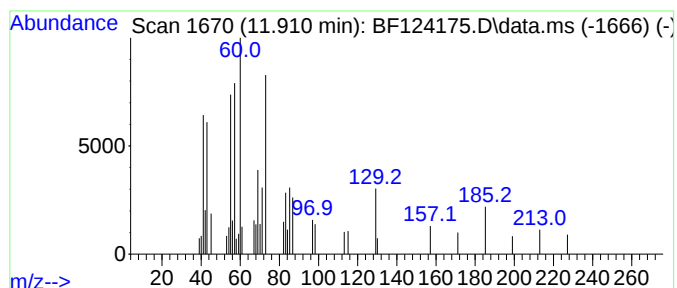
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	2.67 ng	43730	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	53
2			Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	47
3			Undecanoic acid	186	C11H22O2	000112-37-8	47
4			n-Decanoic acid	172	C10H20O2	000334-48-5	47
5			Tridecanoic acid	214	C13H26O2	000638-53-9	47



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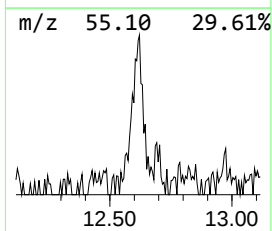
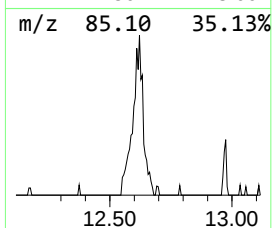
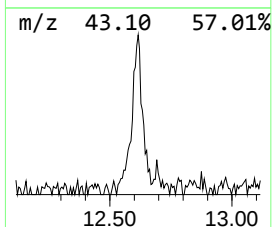
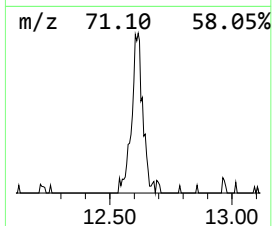
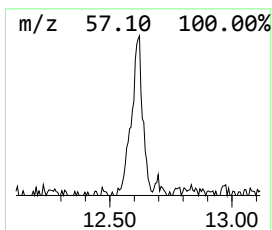
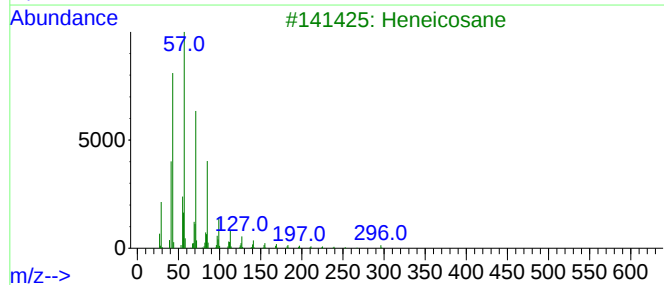
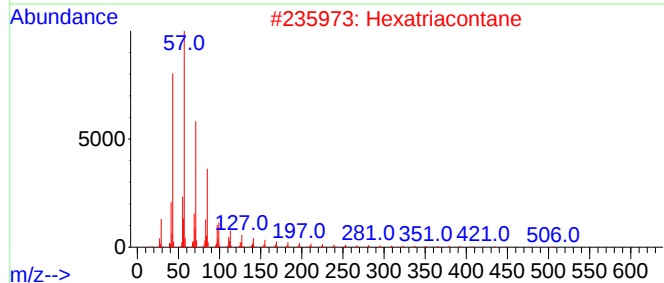
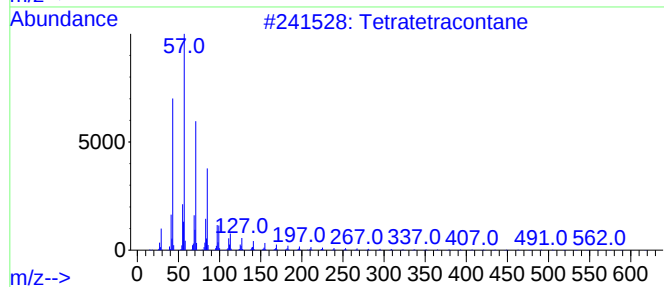
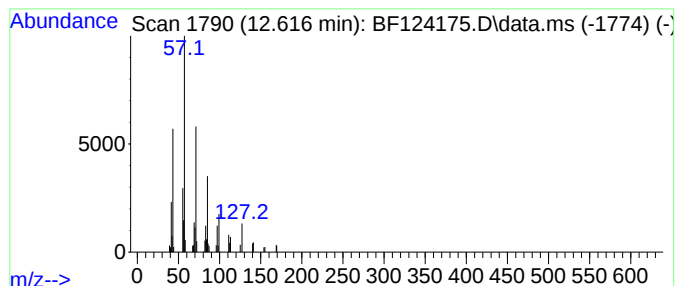
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Peak Number 4 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	13.91 ng	227522	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	80
2			Hexatriacontane	507	C36H74	000630-06-8	80
3			Heneicosane	296	C21H44	000629-94-7	72
4			Octacosane	394	C28H58	000630-02-4	72
5			Heptacosane	380	C27H56	000593-49-7	72



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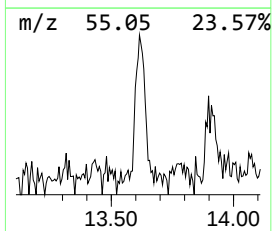
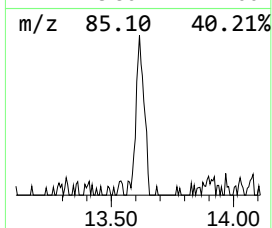
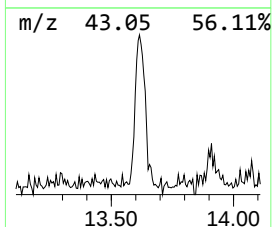
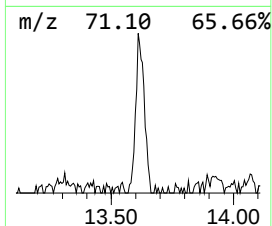
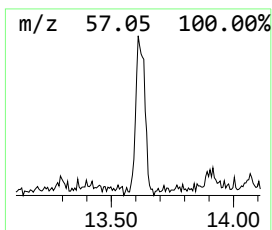
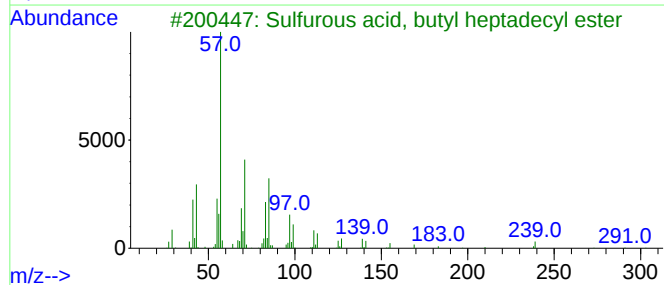
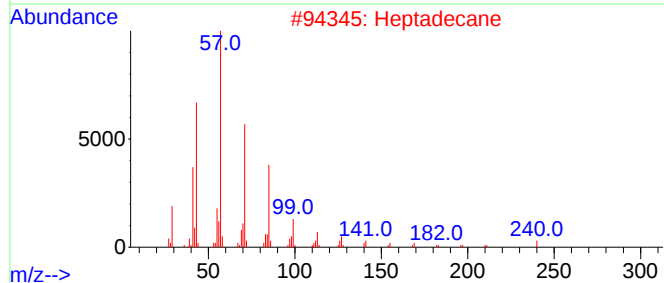
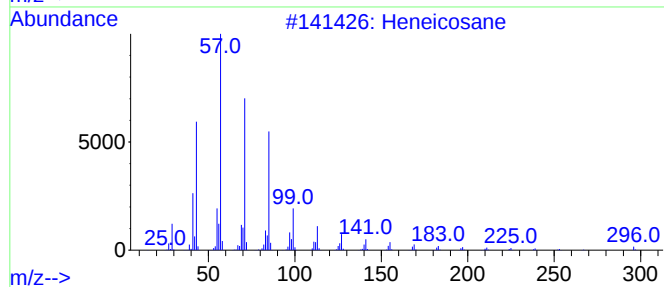
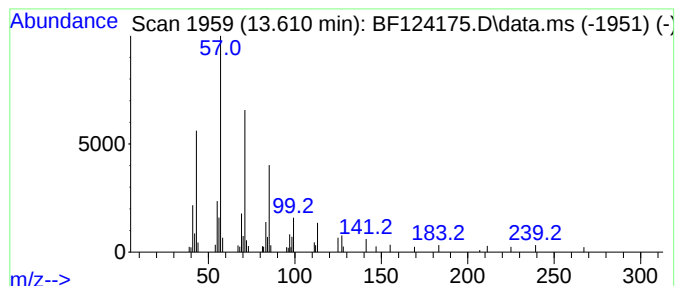
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.610	16.01 ng	198298	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Heptadecane	240	C17H36	000629-78-7	90
3			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	90
4			Hentriacontane	437	C31H64	000630-04-6	87
5			Hexacosane	366	C26H54	000630-01-3	87



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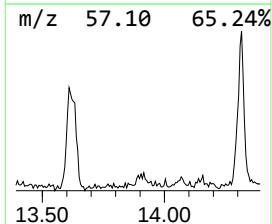
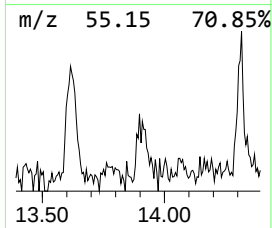
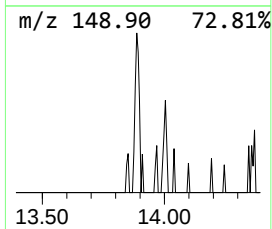
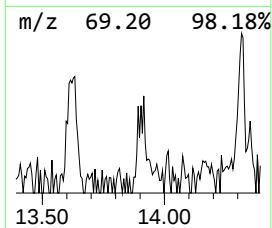
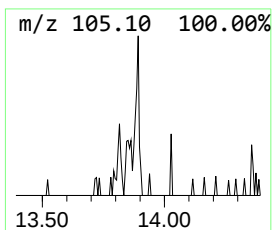
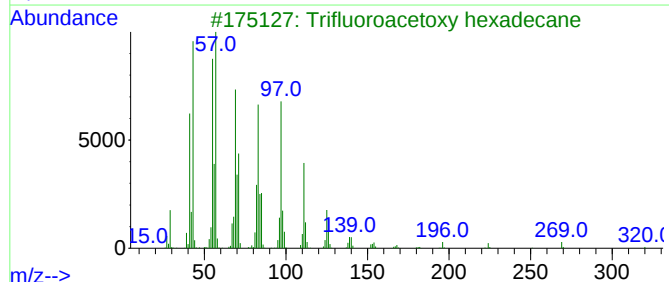
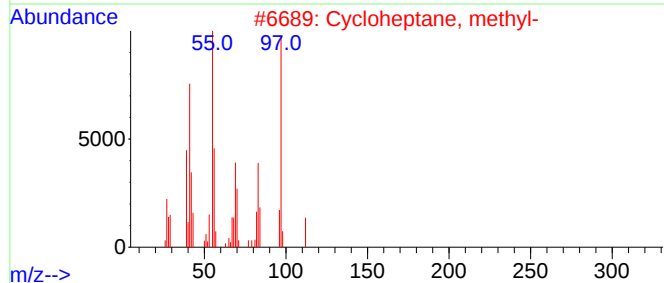
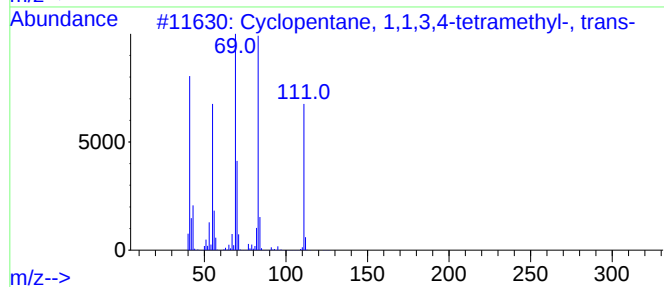
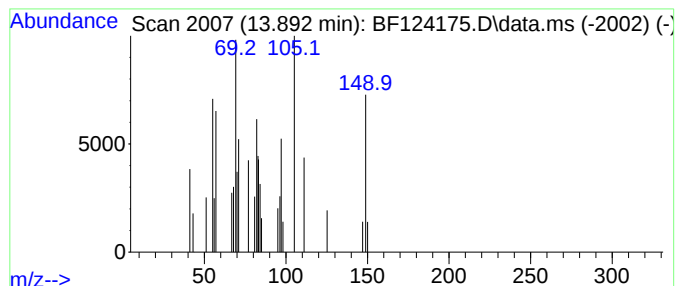
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.892 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.60 ng	56937	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	43
2			Cycloheptane, methyl-	112	C8H16	004126-78-7	43
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	40
4			Cyclohexane, 1,1'-(1,2-dimethyl-...	222	C16H30	054889-87-1	40
5			1-Hexadecanol	242	C16H34O	036653-82-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124175.D
Acq On : 8 Jun 2021 12:09
Operator : JU/CG
Sample : M2613-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(90-94)

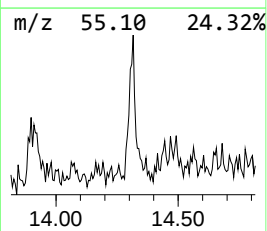
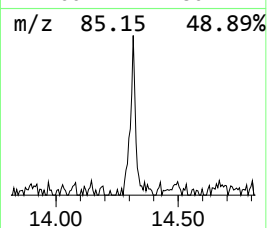
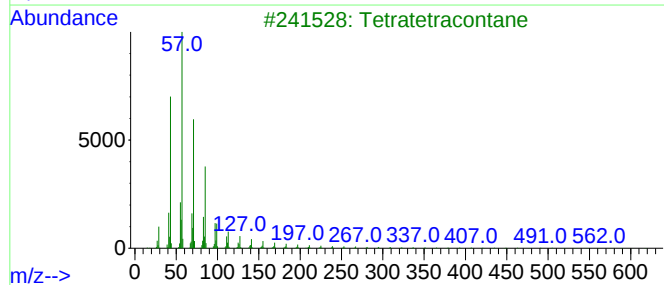
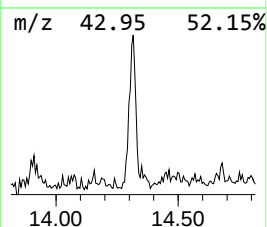
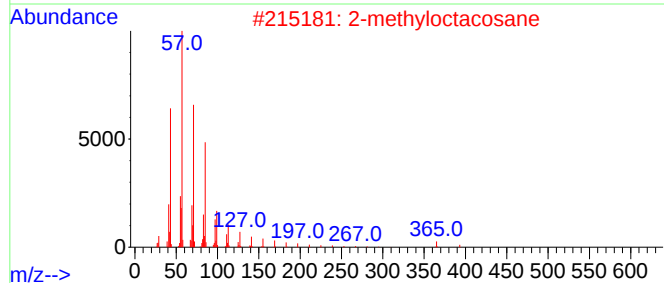
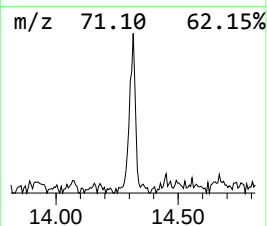
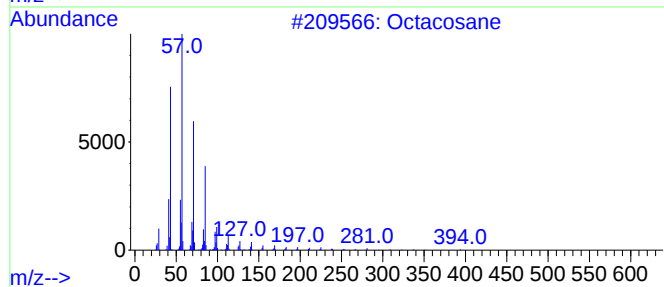
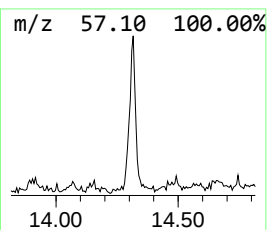
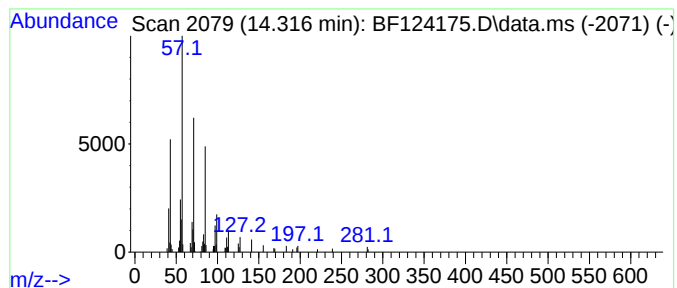
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.316	16.07 ng	199122	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124175.D
Acq On : 8 Jun 2021 12:09
Operator : JU/CG
Sample : M2613-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

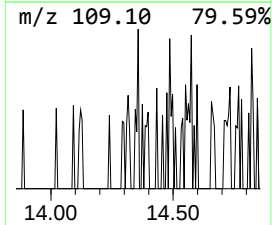
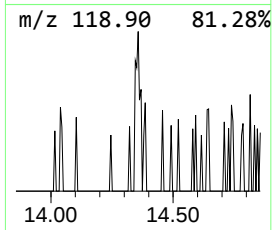
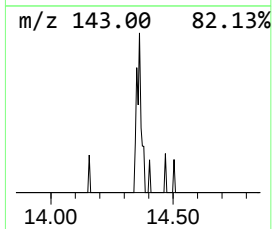
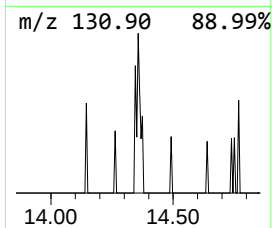
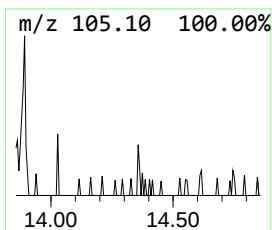
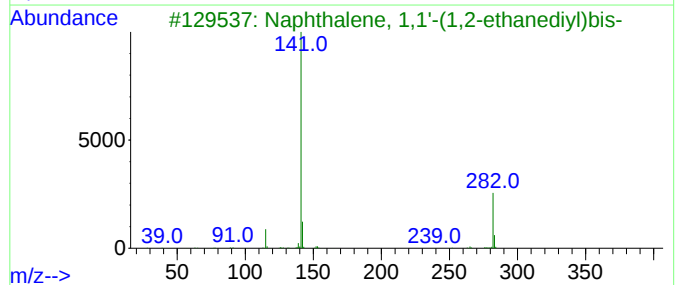
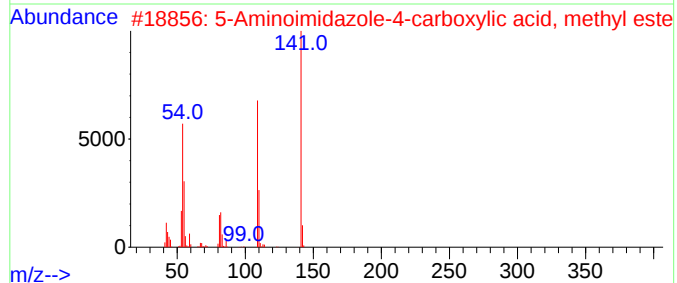
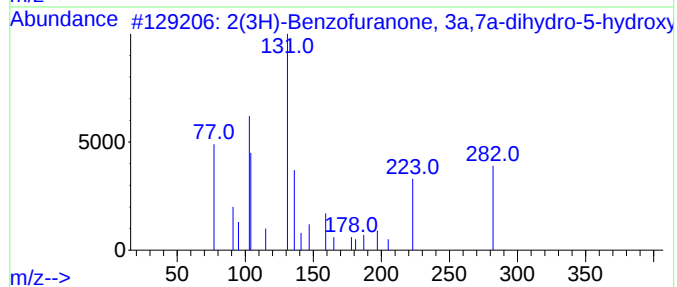
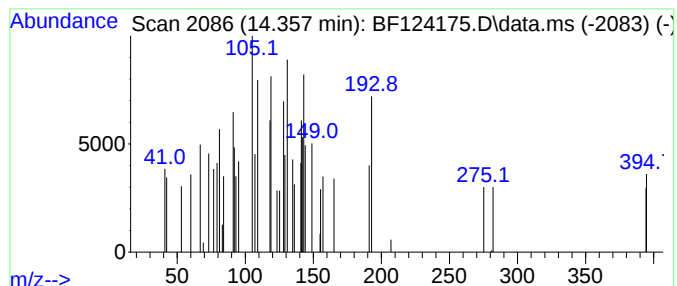
Instrument :
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ClientSampleId :
18-B12(90-94)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.357 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.357	2.46 ng	30477	Chrysene-d12	14.027	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzofuranone, 3a,7a-dihyd...	282	C17H14O4	039012-05-0	10
2	5-Aminoimidazole-4-carboxylic ac...	141	C5H7N3O2	004919-00-0	9
3	Naphthalene, 1,1'-(1,2-ethanedi...	282	C22H18	015374-45-5	9
4	Carbamic acid, N-phenyl-, oxiran...	193	C10H11NO3	027087-14-5	9
5	2-Aminoimidazole-4-carboxylic ac...	141	C5H7N3O2	1000129-59-6	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124175.D
Acq On : 8 Jun 2021 12:09
Operator : JU/CG
Sample : M2613-02
Misc :
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Instrument :
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ClientSampleId :
18-B12(90-94)

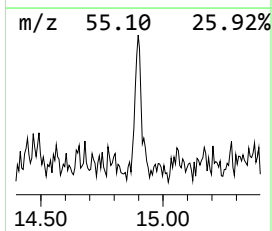
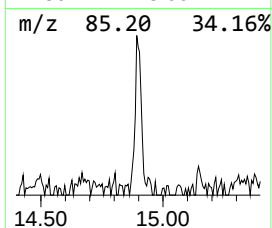
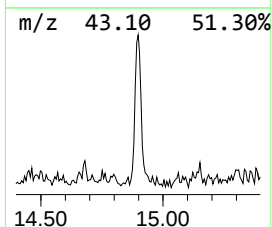
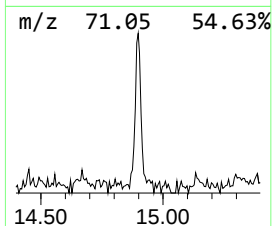
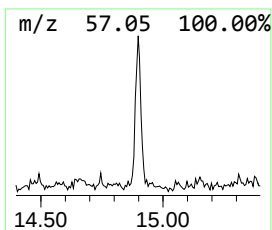
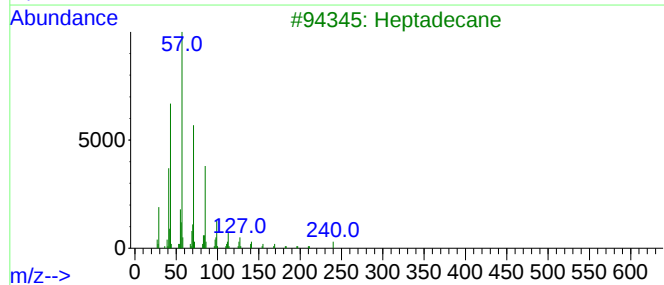
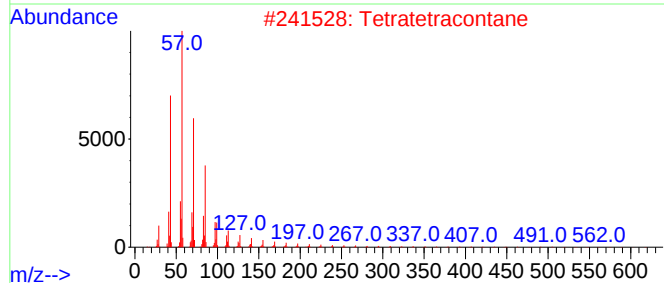
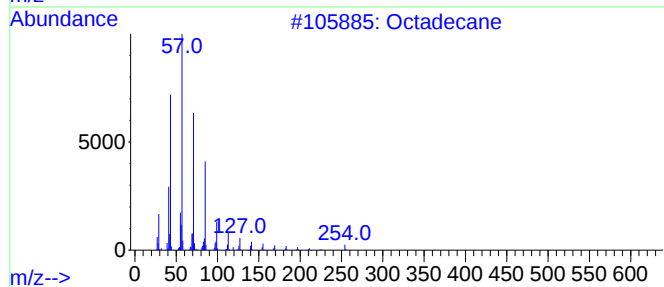
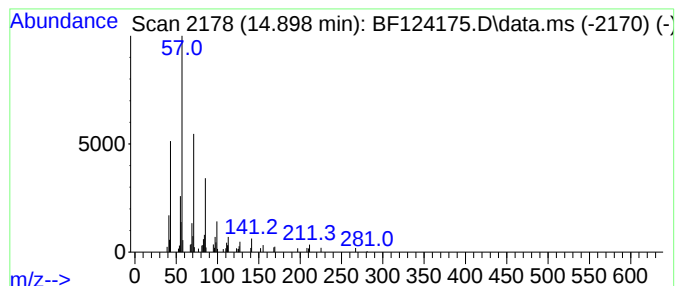
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	15.31 ng	186370	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	87
2			Tetratetracontane	619	C44H90	007098-22-8	87
3			Heptadecane	240	C17H36	000629-78-7	87
4			Hexadecane	226	C16H34	000544-76-3	86
5			Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124175.D
Acq On : 8 Jun 2021 12:09
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Sample : M2613-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
18-B12(90-94)

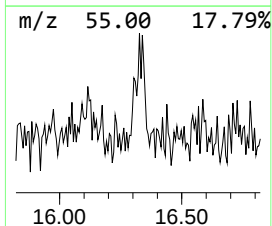
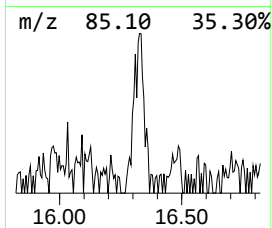
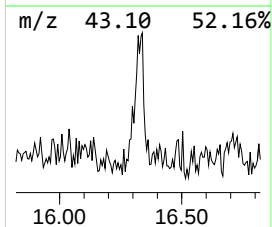
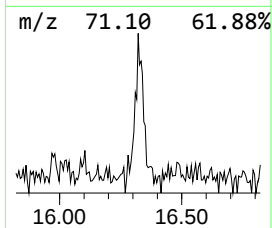
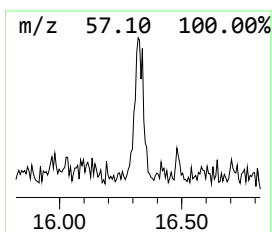
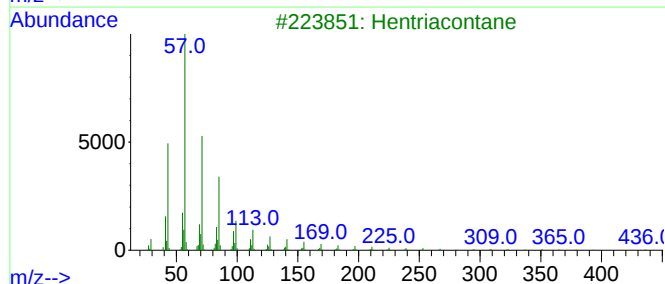
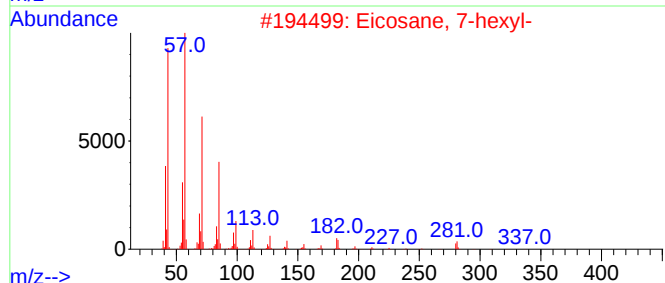
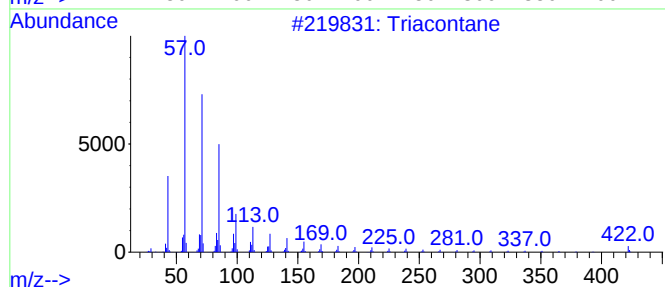
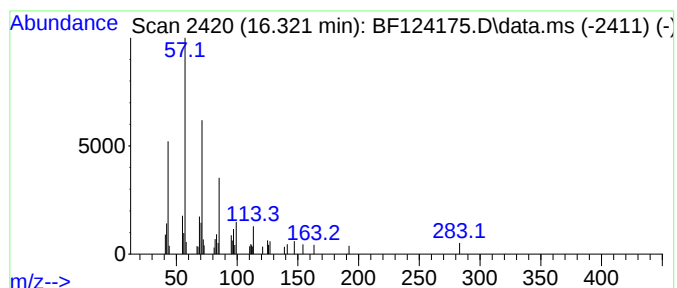
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.321	9.59 ng	116780	Perylene-d12	15.510

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	80
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
3		Hentriacontane	437	C31H64	000630-04-6	80
4		Pentacosane	352	C25H52	000629-99-2	80
5		Hexacosane	366	C26H54	000630-01-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124175.D
Acq On : 8 Jun 2021 12:09
Operator : JU/CG
Sample : M2613-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
18-B12(90-94)

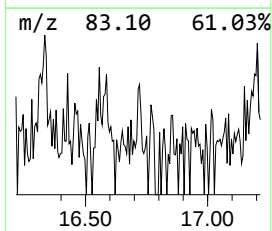
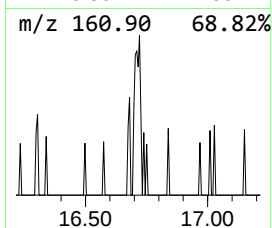
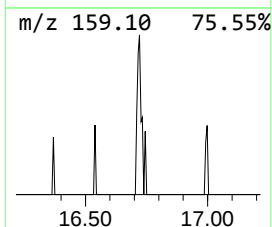
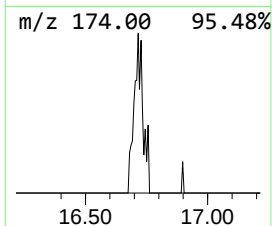
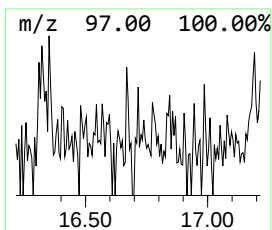
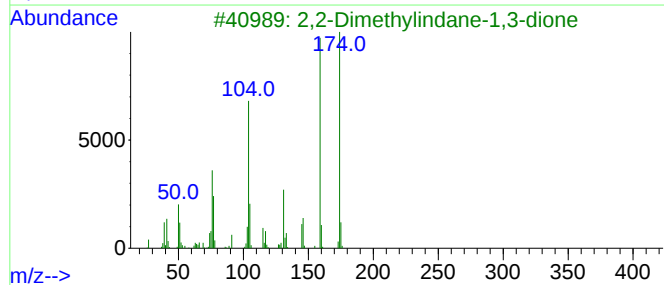
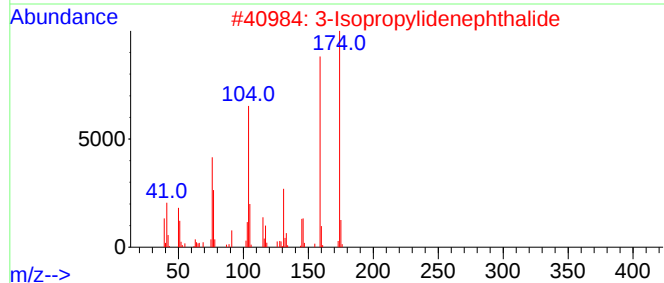
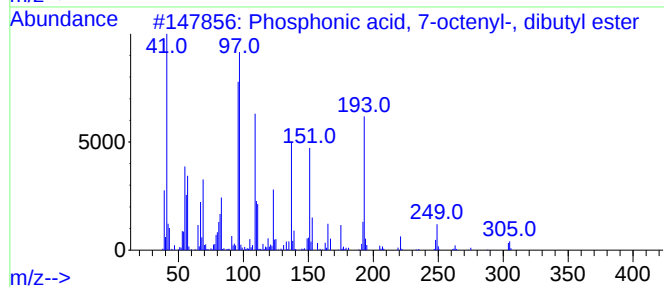
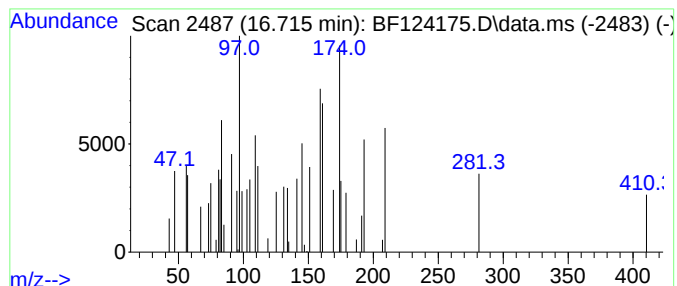
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.715 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.715	2.46 ng	29944	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphonic acid, 7-octenyl-, dib...	304	C16H33O3P	1000115-79-7	14
2			3-Isopropylidenephthalide	174	C11H10O2	004767-54-8	12
3			2,2-Dimethylindane-1,3-dione	174	C11H10O2	017190-77-1	12
4			4-Dimethylaminopyrido[3,2-c]pyri...	174	C9H10N4	1000326-90-5	10
5			2H-Pyrido[1,2-a]pyrimidin-2-one,...	174	C10H10N2O	022365-23-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124175.D
Acq On : 8 Jun 2021 12:09
Operator : JU/CG
Sample : M2613-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

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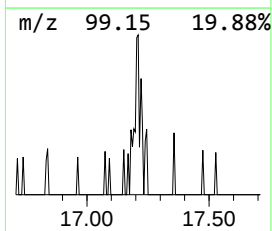
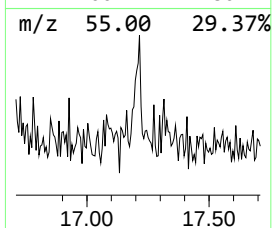
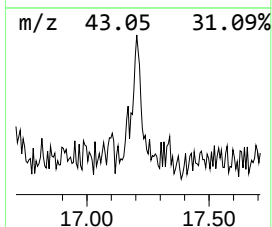
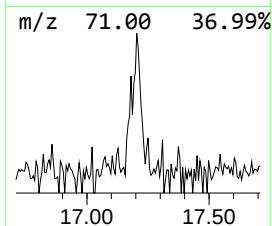
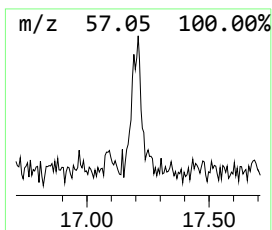
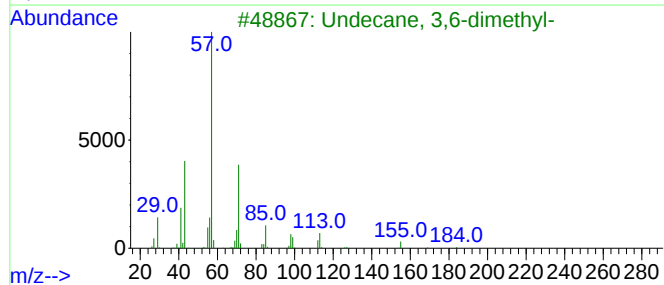
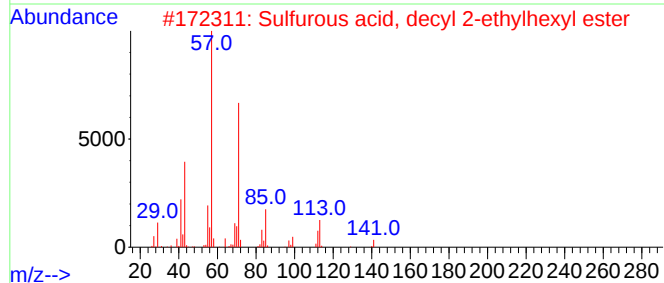
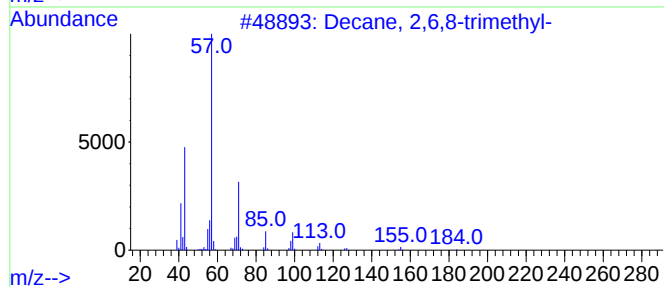
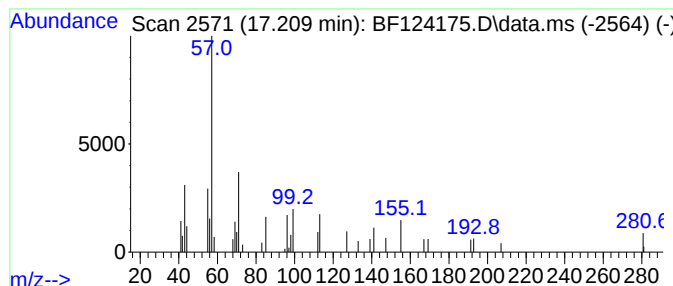
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Decane, 2,6,8-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.209	6.46 ng	78593	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	53
2			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	43
3			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	43
4			Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	43
5			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
Data File : BF124175.D
Acq On : 8 Jun 2021 12:09
Operator : JU/CG
Sample : M2613-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
18-B12(90-94)

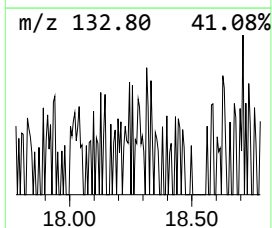
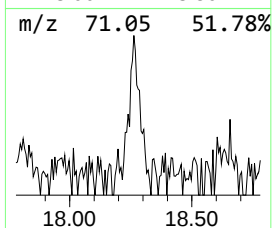
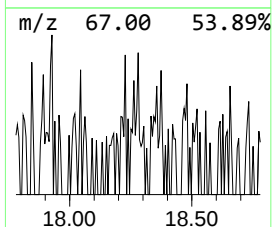
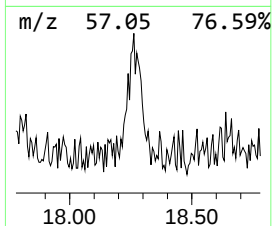
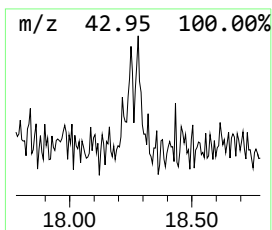
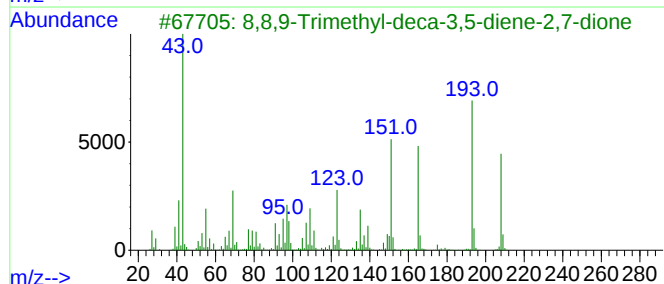
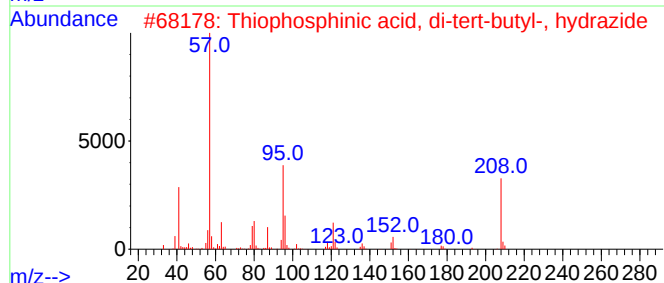
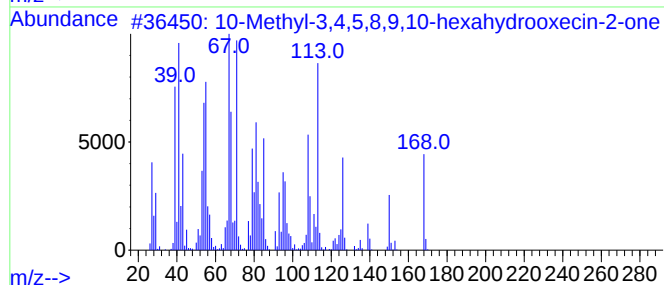
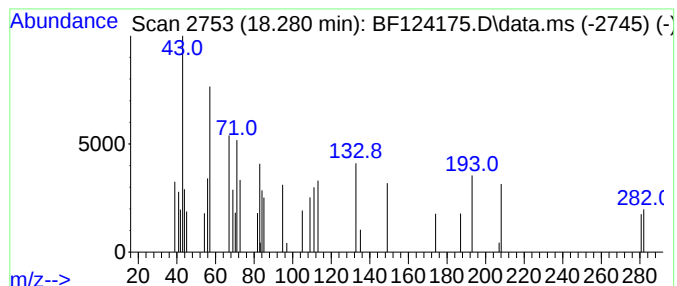
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown18.280 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.280	2.99 ng	36452	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methyl-3,4,5,8,9,10-hexahydro...	168	C10H16O2	136230-43-8	10		
2	Thiophosphinic acid, di-tert-but...	208	C8H21N2PS	1000296-42-0	9		
3	8,8,9-Trimethyl-deca-3,5-diene-2...	208	C13H20O2	1000194-25-9	9		
4	2,5,5,6,8a-Pentamethyl-trans-4a,...	208	C14H24O	1000215-77-8	9		
5	4,5-Heptadien-2-ol, 3,3,6-trimet...	154	C10H18O	060432-69-1	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
 Data File : BF124175.D
 Acq On : 8 Jun 2021 12:09
 Operator : JU/CG
 Sample : M2613-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 18-B12(90-94)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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...	2.128	71.3	ng	726387	1	6.857	203735	20.0
unknown8.045	8.045	2.4	ng	30761	2	8.140	259785	20.0
Dodecanoic acid	11.910	2.7	ng	43730	4	11.386	327209	20.0
Tetratetracontane	12.616	13.9	ng	227522	4	11.386	327209	20.0
Heneicosane	13.610	16.0	ng	198298	5	14.027	247778	20.0
unknown13.892	13.892	4.6	ng	56937	5	14.027	247778	20.0
Octacosane	14.316	16.1	ng	199122	5	14.027	247778	20.0
unknown14.357	14.357	2.5	ng	30477	5	14.027	247778	20.0
Octadecane	14.898	15.3	ng	186370	6	15.510	243500	20.0
Triacontane	16.321	9.6	ng	116780	6	15.510	243500	20.0
unknown16.715	16.715	2.5	ng	29944	6	15.510	243500	20.0
Decane, 2,6,8-t...	17.209	6.5	ng	78593	6	15.510	243500	20.0
unknown18.280	18.280	3.0	ng	36452	6	15.510	243500	20.0