

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081320\
 Data File : BF121278.D
 Acq On : 13 Aug 2020 19:06
 Operator : JU/CG
 Sample : L3659-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP1-3

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF081320.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.899	475	478	487	rVB	27862	35542	1.50%	0.226%
2	5.322	546	550	564	rBV	1710499	1601945	67.49%	10.194%
3	6.357	722	726	745	rBV	1814316	1617924	68.17%	10.296%
4	6.722	784	788	791	rBV	536877	479880	20.22%	3.054%
5	7.281	879	883	887	rBV	1188699	1104058	46.52%	7.026%
6	8.004	1002	1006	1009	rBV	830916	634180	26.72%	4.036%
7	9.081	1185	1189	1192	rBV	2344228	2106457	88.75%	13.405%
8	9.469	1253	1255	1259	rVB	109284	88547	3.73%	0.563%
9	9.751	1300	1303	1307	rVB	934527	727913	30.67%	4.632%
10	10.539	1433	1437	1449	rBV	1461886	1277617	53.83%	8.130%
11	11.233	1551	1555	1559	rBV	1012208	782029	32.95%	4.976%
12	12.757	1811	1814	1817	rVB	62632	50478	2.13%	0.321%
13	12.822	1821	1825	1828	rBV	2669834	2373489	100.00%	15.104%
14	13.580	1951	1954	1958	rBV	159855	120525	5.08%	0.767%
15	13.739	1976	1981	1999	rBV2	143779	398684	16.80%	2.537%
16	13.869	1999	2003	2006	rVV	889162	755965	31.85%	4.811%
17	14.345	2077	2084	2087	rBV2	28631	31015	1.31%	0.197%
18	14.386	2087	2091	2102	rVV6	23670	70919	2.99%	0.451%
19	14.639	2128	2134	2140	rVB2	27380	35848	1.51%	0.228%
20	14.963	2185	2189	2194	rBV	81227	89817	3.78%	0.572%
21	15.033	2195	2201	2207	rBV8	16774	38198	1.61%	0.243%
22	15.286	2238	2244	2247	rBV	602368	685607	28.89%	4.363%
23	15.315	2247	2249	2257	rVB	41736	48702	2.05%	0.310%
24	15.721	2313	2318	2325	rBV	102827	150363	6.34%	0.957%
25	15.833	2328	2337	2342	rBV8	26010	80186	3.38%	0.510%
26	16.192	2393	2398	2409	rVB3	41331	80725	3.40%	0.514%
27	16.457	2439	2443	2450	rVB8	14765	28124	1.18%	0.179%
28	16.739	2485	2491	2498	rBV	41246	81996	3.45%	0.522%
29	17.380	2597	2600	2609	rVB4	28975	62372	2.63%	0.397%
30	18.139	2724	2729	2744	rVB6	24829	75398	3.18%	0.480%

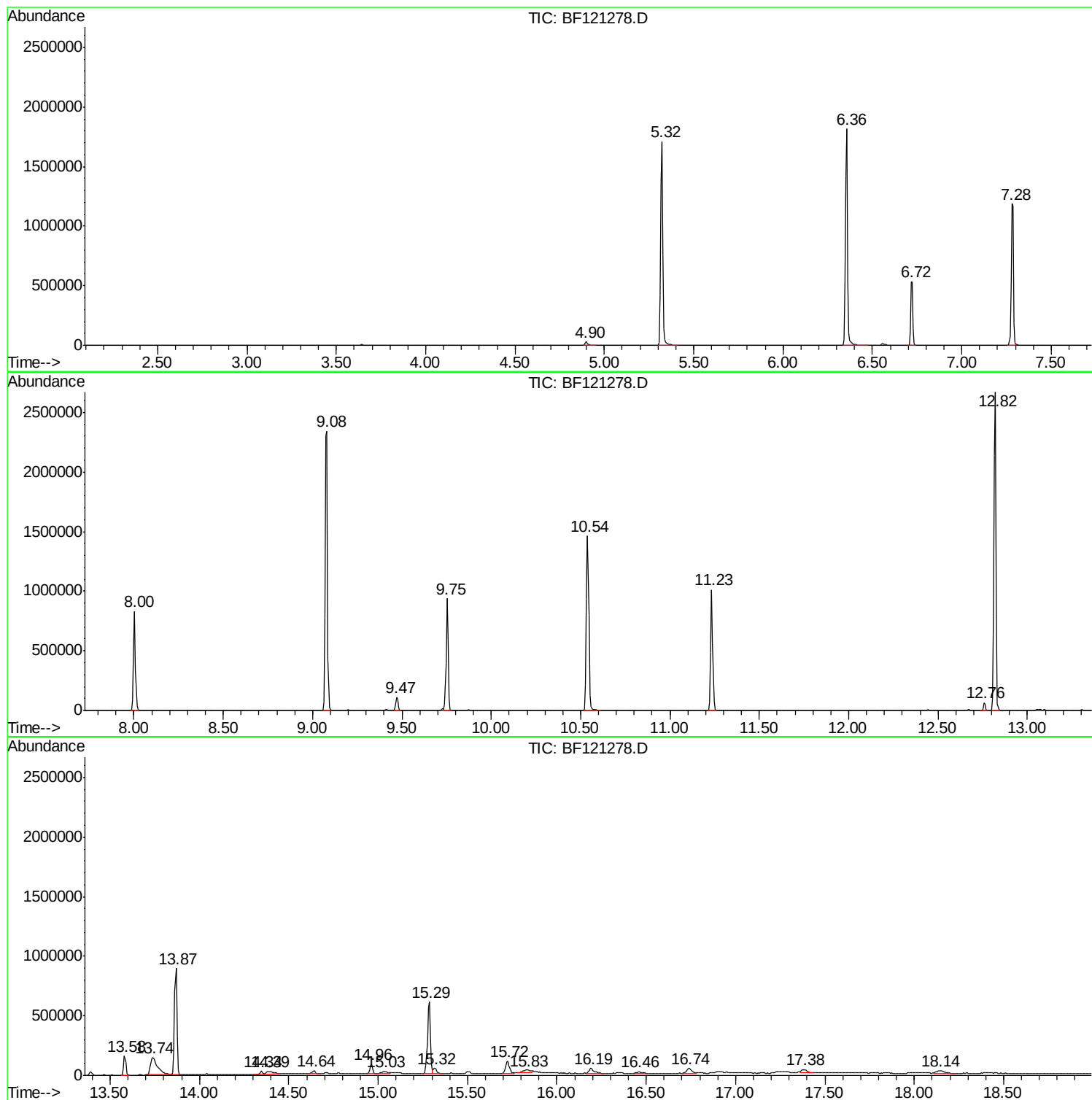
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF081320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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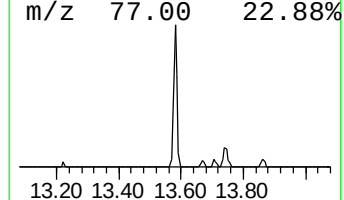
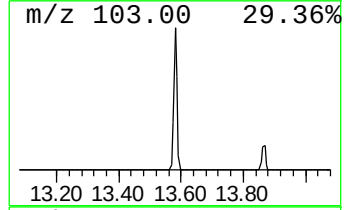
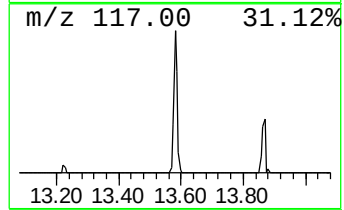
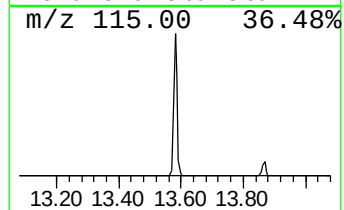
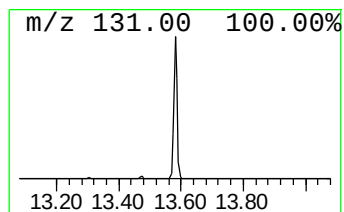
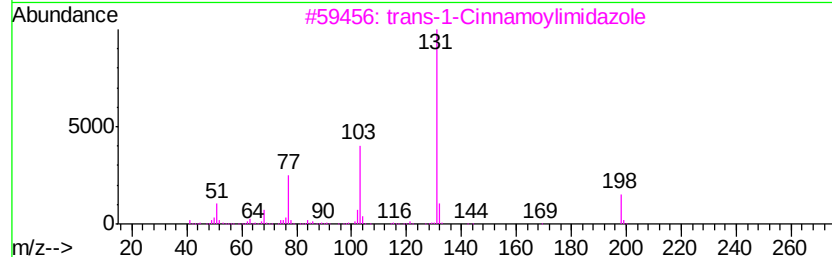
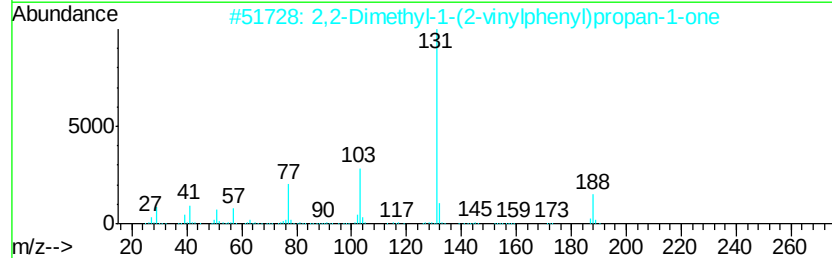
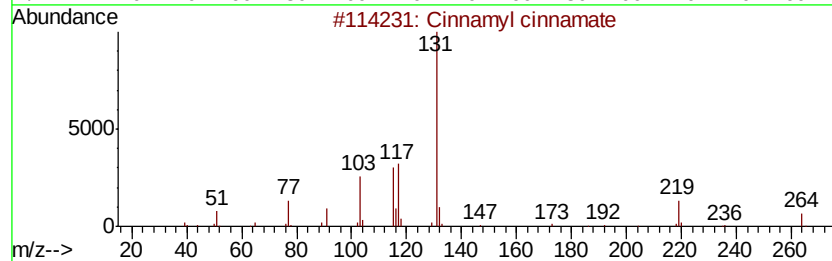
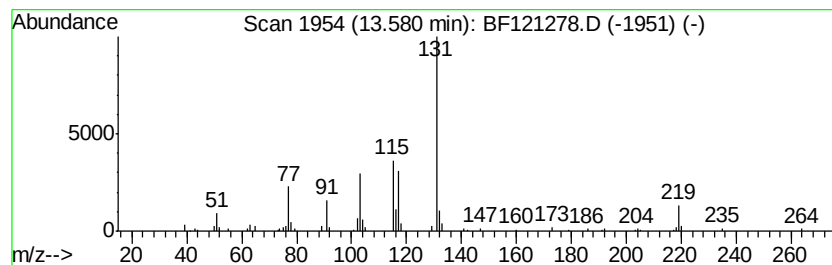
Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF081320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cinnamyl cinnamate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.58	3.19 ng	120525	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
2	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
3	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	50
4	2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	50
5	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	50



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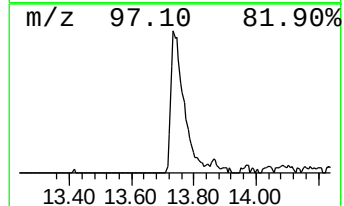
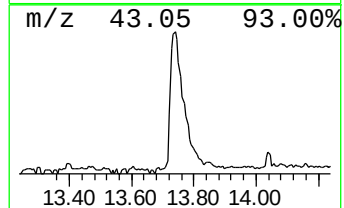
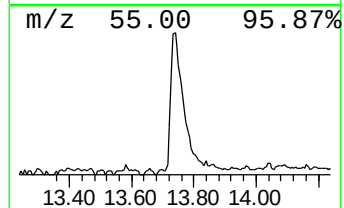
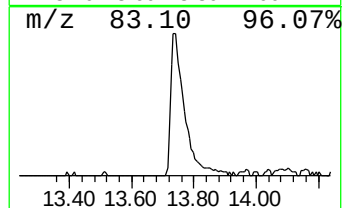
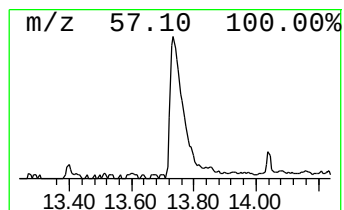
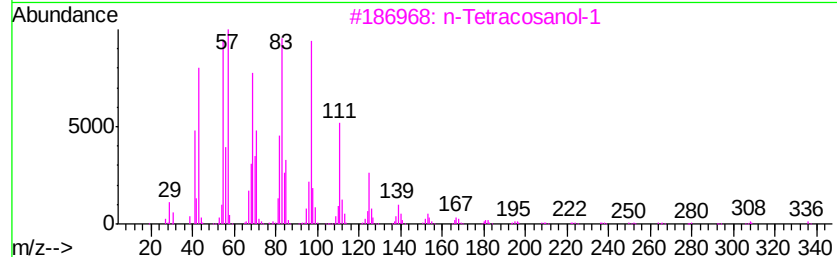
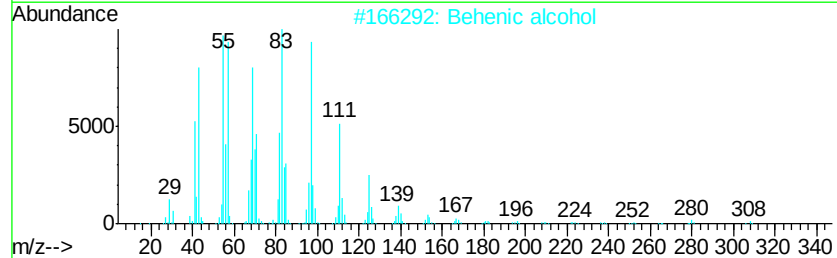
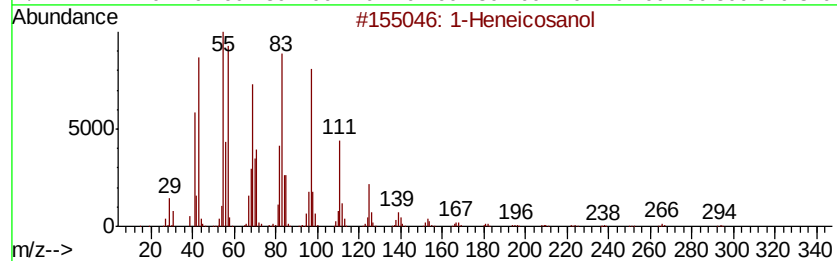
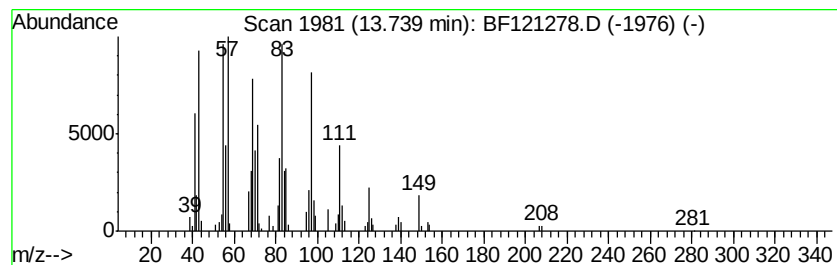
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.74	10.55 ng	398684	Chrysene-d12		13.87
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	1-Nonadecene	266	C19H38	018435-45-5	91



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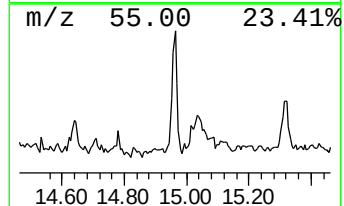
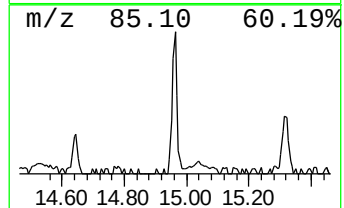
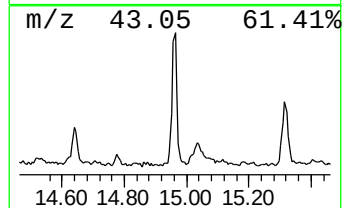
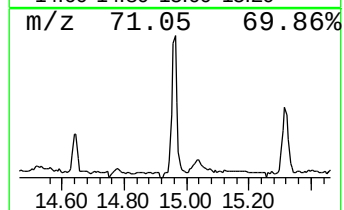
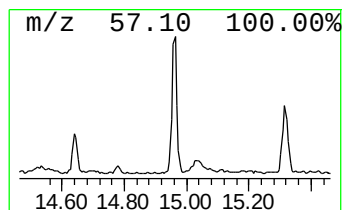
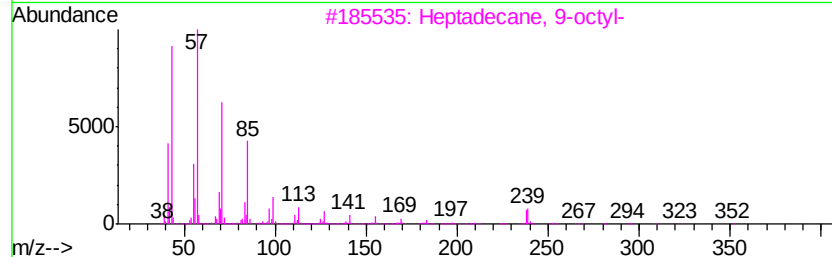
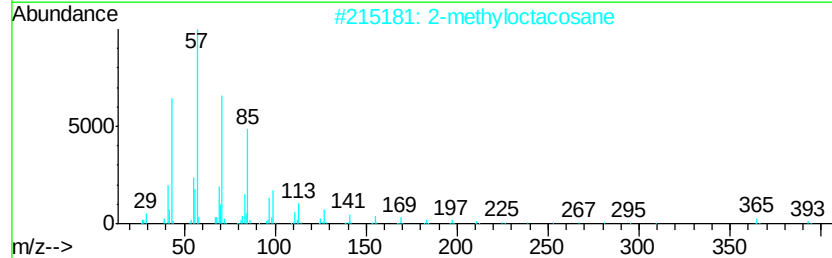
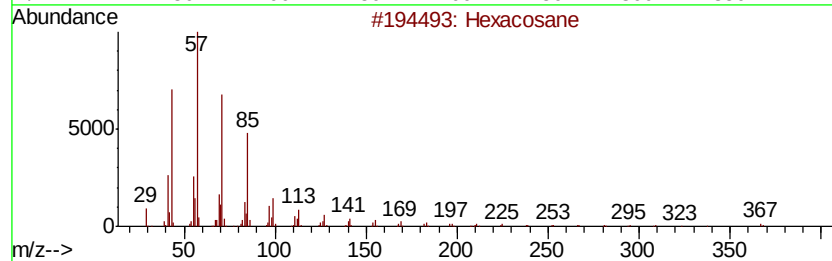
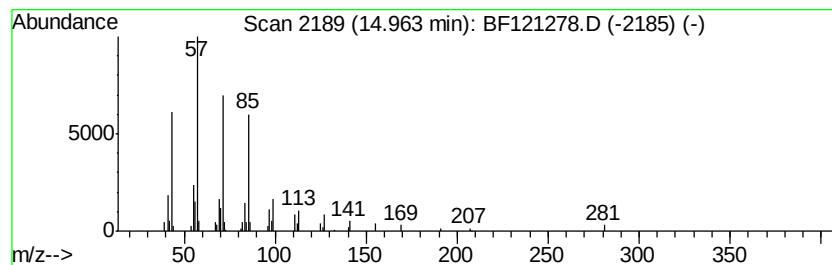
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.62 ng	89817	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Heneicosane		296	C21H44	000629-94-7	91
5	Heptacosane		380	C27H56	000593-49-7	91



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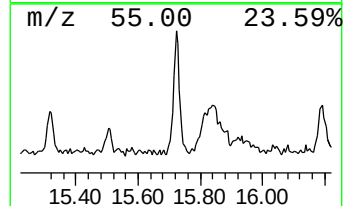
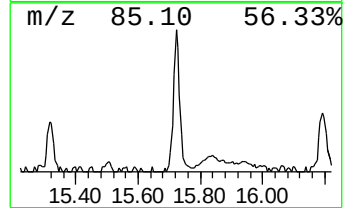
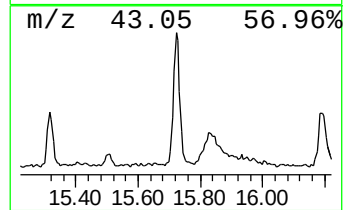
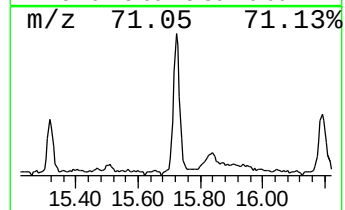
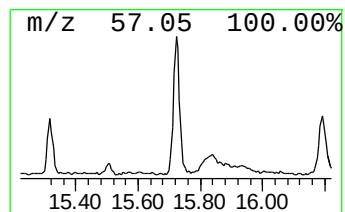
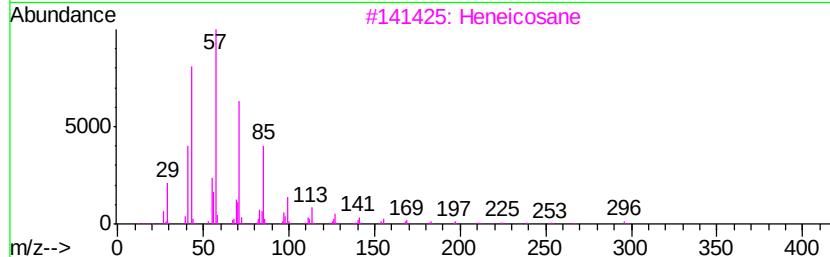
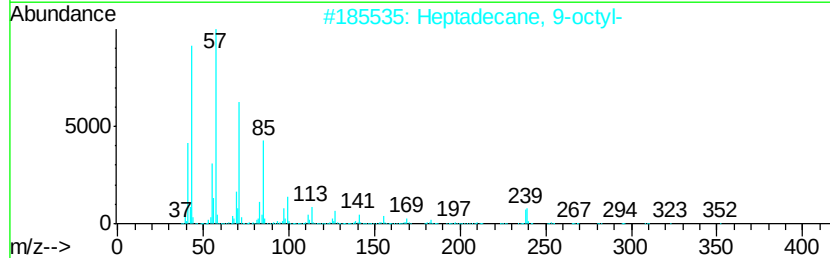
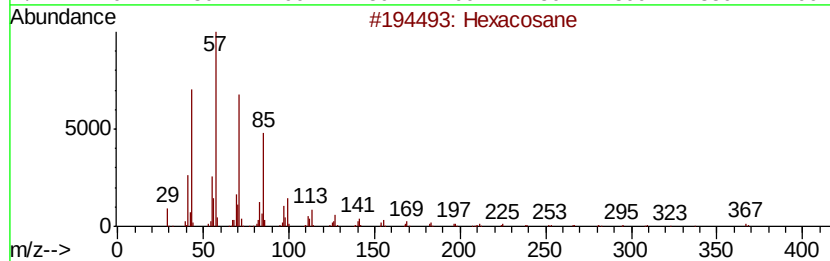
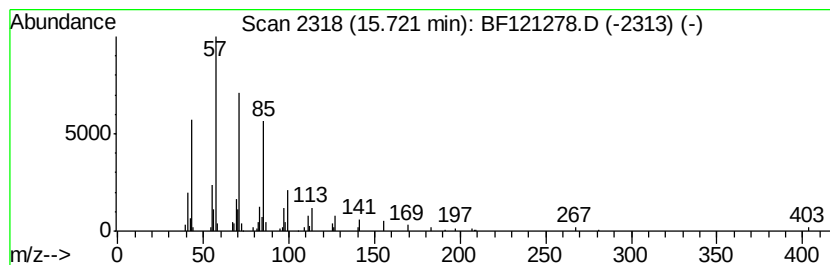
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptadecane, 9-octyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.72	4.39 ng	150363	Perylene-d12	15.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



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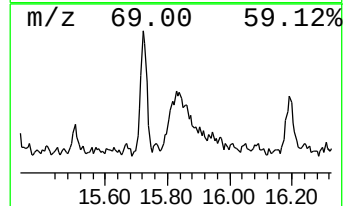
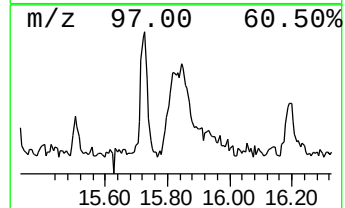
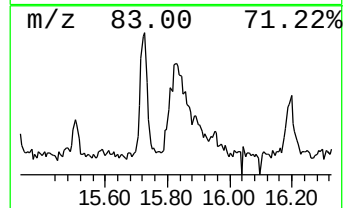
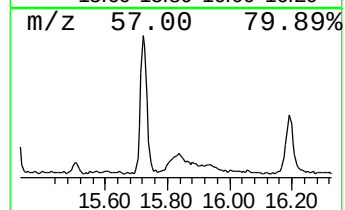
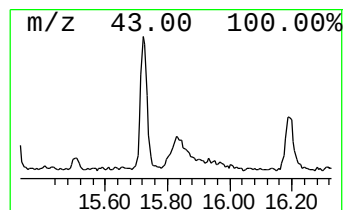
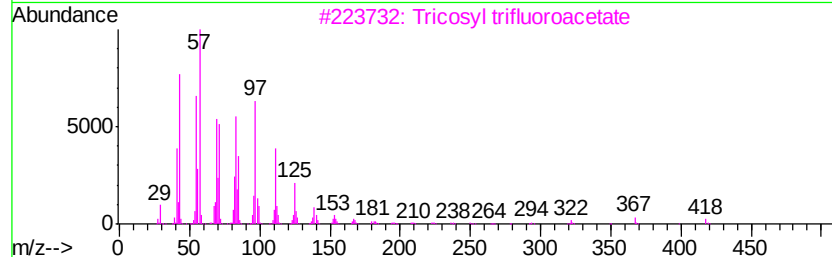
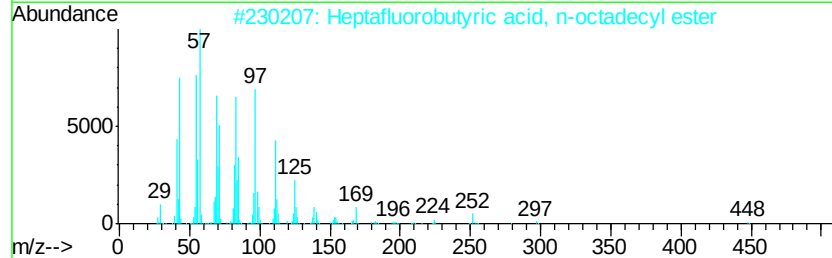
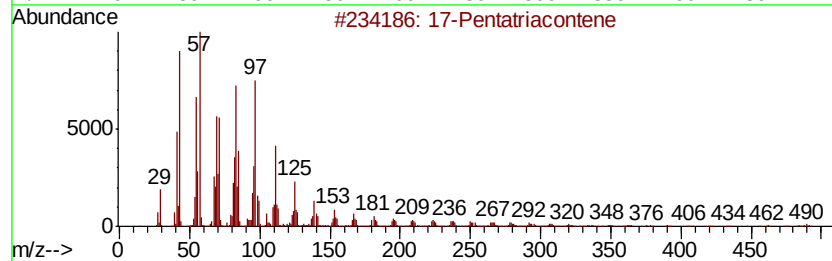
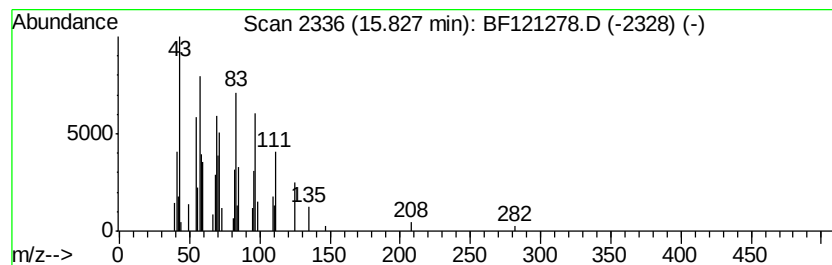
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	2.34 ng	80186	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	17-Pentatriacontene	491 C35H70	006971-40-0	70
2	Heptafluorobutyric acid, n-octad...	466 C22H37F7O2	000400-57-7	64
3	Tricosyl trifluoroacetate	436 C25H47F3O2	1000351-75-1	64
4	Nonadecyl pentafluoropropionate	430 C22H39F5O2	1000351-88-8	64
5	Eicosyl heptafluorobutyrate	494 C24H41F7O2	1000351-83-5	64



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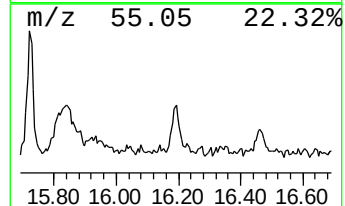
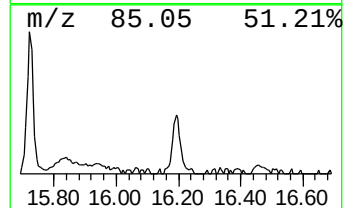
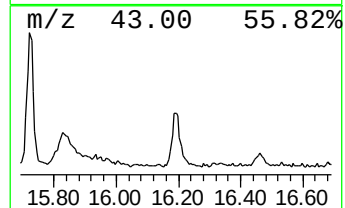
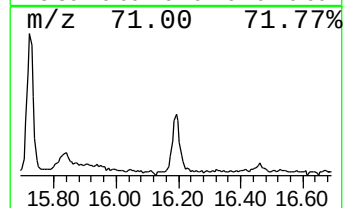
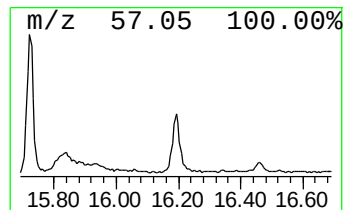
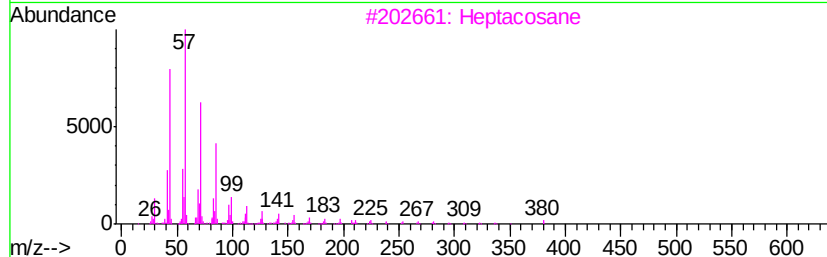
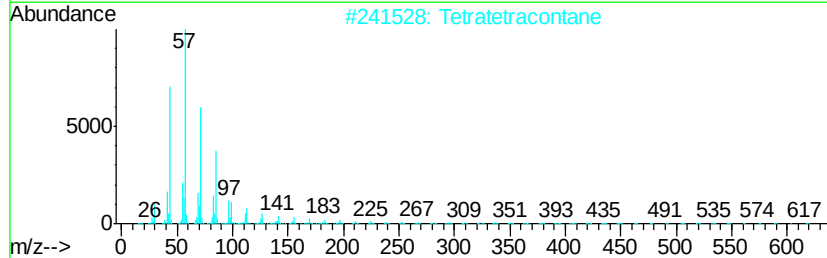
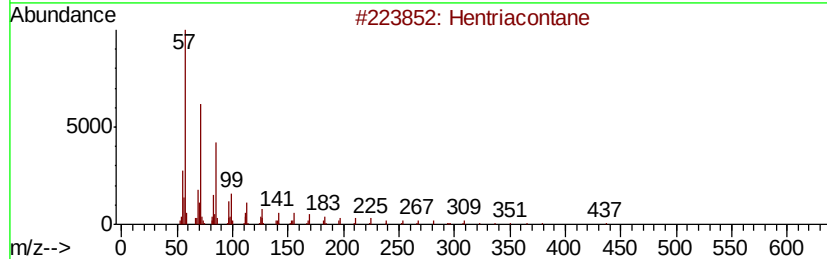
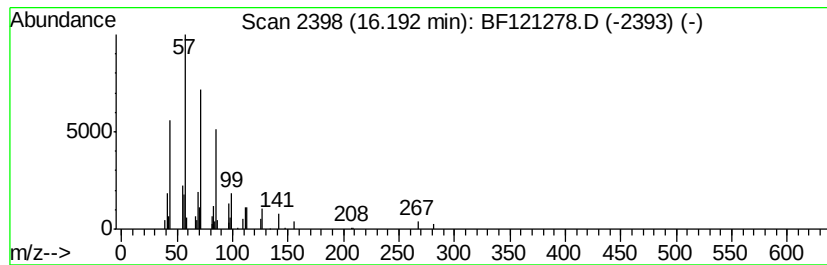
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.35 ng	80725	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	90
2	Tetratetracontane		619	C44H90	007098-22-8	90
3	Heptacosane		380	C27H56	000593-49-7	90
4	Octacosane		394	C28H58	000630-02-4	90
5	Hexacosane		366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081320\
 Data File : BF121278.D
 Acq On : 13 Aug 2020 19:06
 Operator : JU/CG
 Sample : L3659-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP1-3

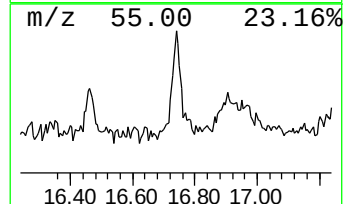
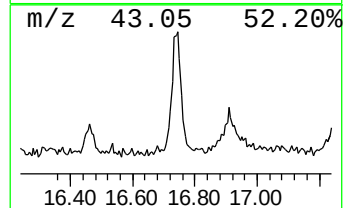
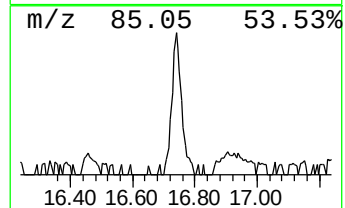
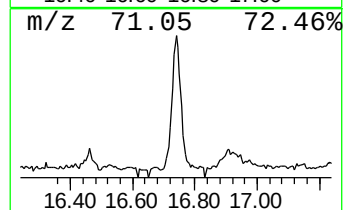
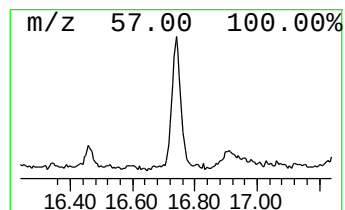
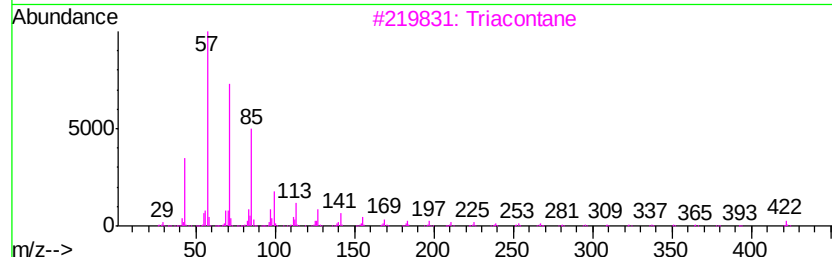
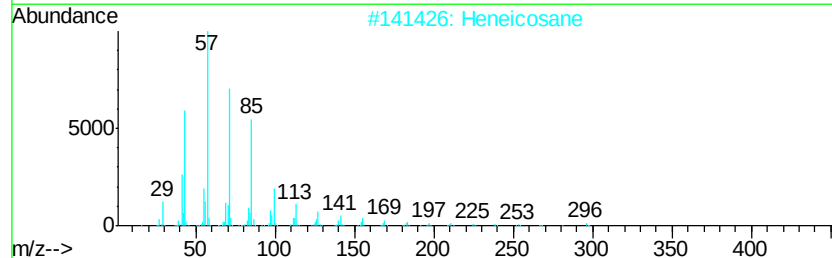
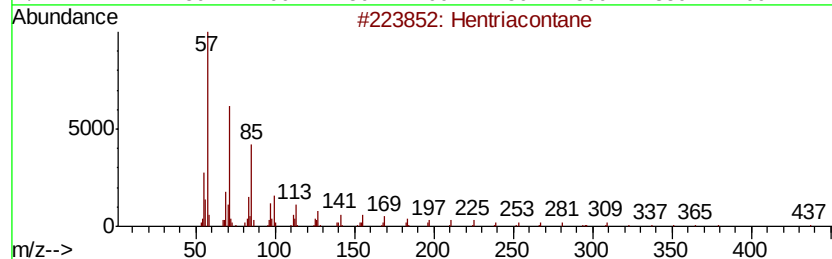
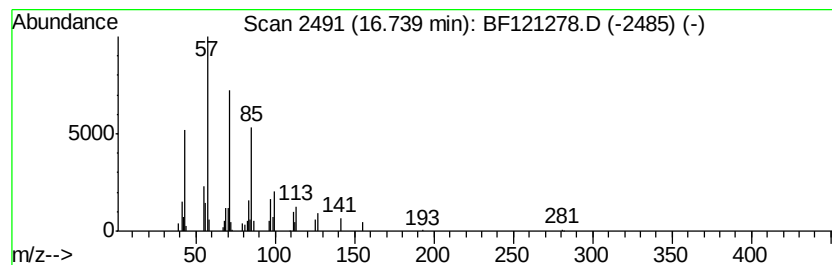
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	2.39 ng	81996	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Triacontane	422	C30H62	000638-68-6	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081320\
Data File : BF121278.D
Acq On : 13 Aug 2020 19:06
Operator : JU/CG
Sample : L3659-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP1-3

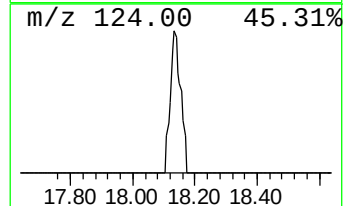
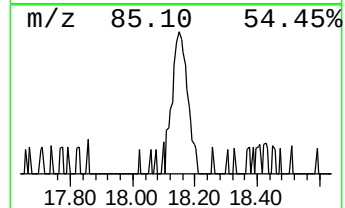
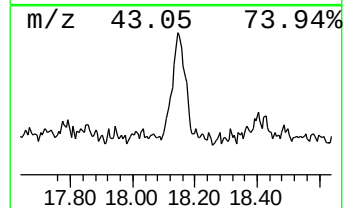
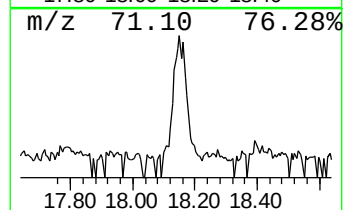
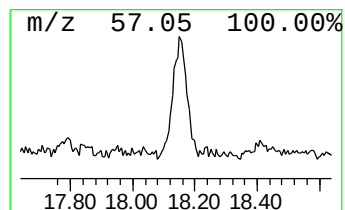
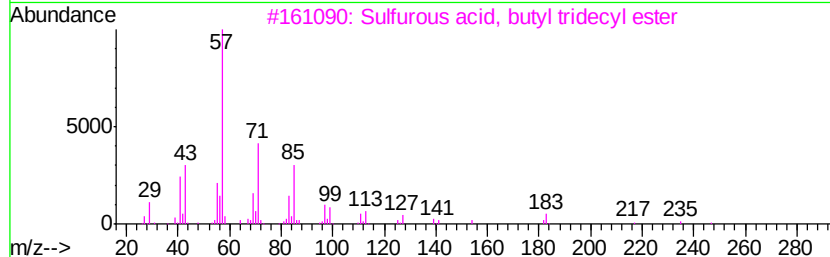
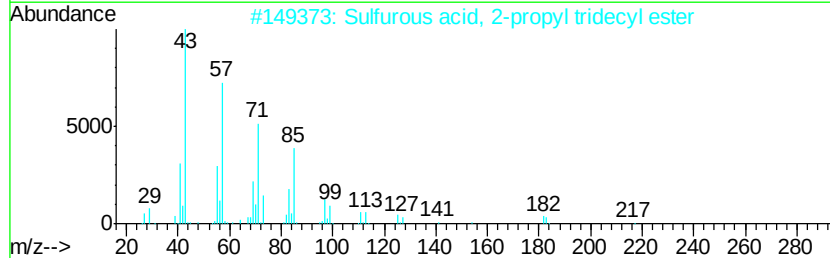
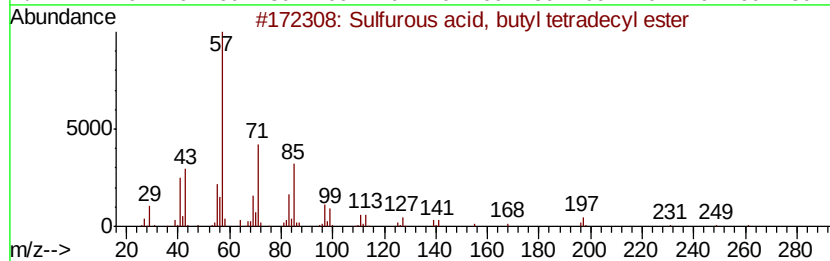
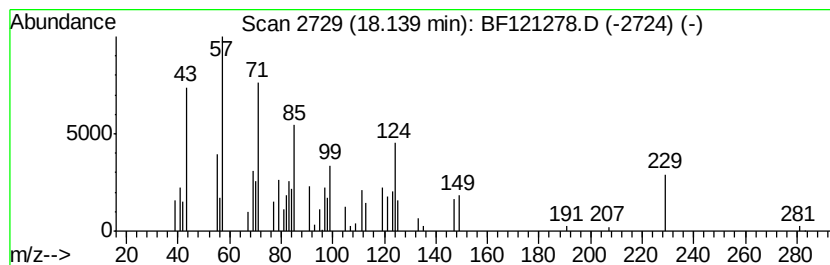
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.14 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.14	2.20 ng	75398	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	43
2		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	43
3		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	43
4		Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	38
5		Tetratetracontane	619	C44H90	007098-22-8	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081320\
Data File : BF121278.D
Acq On : 13 Aug 2020 19:06
Operator : JU/CG
Sample : L3659-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081320.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
Cinnamyl cinnamate	13.58	3.2	ng	120525	5	13.87	755965	20.0
1-Heneicosanol	13.74	10.6	ng	398684	5	13.87	755965	20.0
Hexacosane	14.96	2.6	ng	89817	6	15.29	685607	20.0
Heptadecane, 9-oc...	15.72	4.4	ng	150363	6	15.29	685607	20.0
17-Pentatriacontene	15.83	2.3	ng	80186	6	15.29	685607	20.0
Hentriacontane	16.19	2.4	ng	80725	6	15.29	685607	20.0
Heneicosane	16.74	2.4	ng	81996	6	15.29	685607	20.0
unknown18.14	18.14	2.2	ng	75398	6	15.29	685607	20.0