

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
 Data File : BF117627.D
 Acq On : 30 Oct 2019 16:25
 Operator : JU
 Sample : K5541-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 154-24-(0-2)

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-BF101819.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	5.357	553	556	577	rBV	516476	719906	85.06%	10.062%
2	6.387	728	731	748	rBV	645868	834542	98.60%	11.665%
3	6.504	748	751	765	rVB	885443	846377	100.00%	11.830%
4	6.728	785	789	798	rBV	221890	209880	24.80%	2.934%
5	6.881	812	815	830	rBV	626910	574349	67.86%	8.028%
6	7.292	882	885	905	rBV	363363	470622	55.60%	6.578%
7	8.010	1004	1007	1025	rBV	210176	260215	30.74%	3.637%
8	9.081	1186	1189	1208	rBV	657414	641761	75.82%	8.970%
9	9.481	1254	1257	1272	rBB	69117	75419	8.91%	1.054%
10	9.763	1301	1305	1320	rBB	267681	280010	33.08%	3.914%
11	10.557	1437	1440	1455	rBV	320364	361316	42.69%	5.050%
12	11.251	1554	1558	1561	rBV	217178	228208	26.96%	3.190%
13	11.275	1561	1562	1567	rVB	49391	37921	4.48%	0.530%
14	11.775	1645	1647	1654	rVB4	19942	24957	2.95%	0.349%
15	12.469	1762	1765	1770	rBV	72929	76243	9.01%	1.066%
16	12.698	1798	1804	1810	rBV	66053	80620	9.53%	1.127%
17	12.827	1822	1826	1833	rBV	558236	474423	56.05%	6.631%
18	13.257	1896	1899	1903	rBV3	12324	12585	1.49%	0.176%
19	13.298	1903	1906	1911	rVV2	15908	16669	1.97%	0.233%
20	13.739	1976	1981	1991	rVB5	41808	85700	10.13%	1.198%
21	13.857	1998	2001	2003	rBV	8983	8844	1.04%	0.124%
22	13.892	2003	2007	2011	rVV2	218875	268873	31.77%	3.758%
23	13.921	2011	2012	2019	rVB	40413	28426	3.36%	0.397%
24	14.039	2029	2032	2035	rBV3	9492	12529	1.48%	0.175%
25	14.345	2081	2084	2086	rBV4	10904	9312	1.10%	0.130%
26	14.380	2086	2090	2096	rVV6	15478	27841	3.29%	0.389%
27	14.639	2132	2134	2137	rBV2	15745	14959	1.77%	0.209%
28	14.710	2142	2146	2149	rBV	92007	84100	9.94%	1.175%
29	14.933	2180	2184	2185	rBV2	24007	29438	3.48%	0.411%
30	14.957	2185	2188	2193	rVB3	41414	47426	5.60%	0.663%
31	15.027	2198	2200	2208	rVB6	15557	26663	3.15%	0.373%
32	15.221	2229	2233	2235	rBV	15344	18988	2.24%	0.265%
33	15.280	2240	2243	2246	rVV	20783	26942	3.18%	0.377%
34	15.333	2246	2252	2261	rVB	132941	203577	24.05%	2.845%

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154-24-(0-2)

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.715	2313	2317	2323	rVB2	23996	34904	4.12%	0.488%
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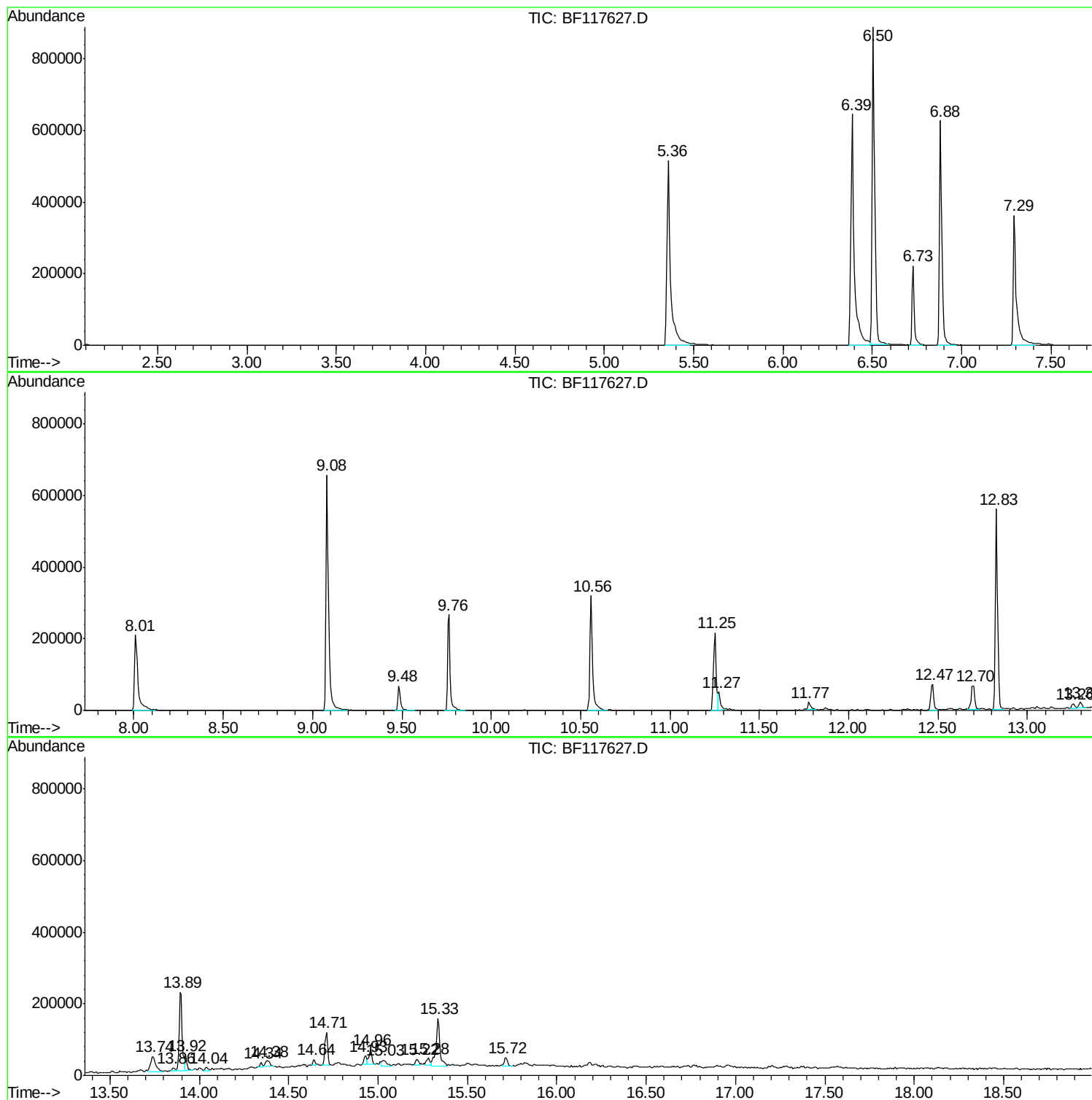
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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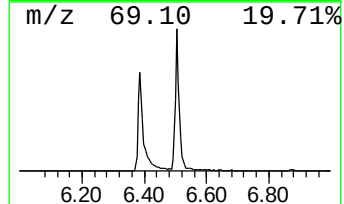
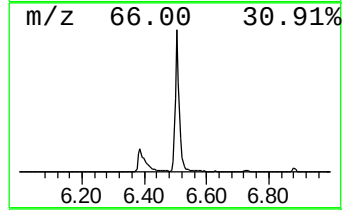
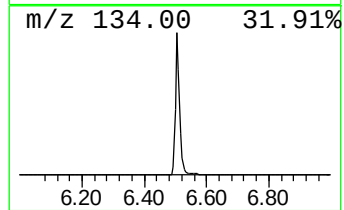
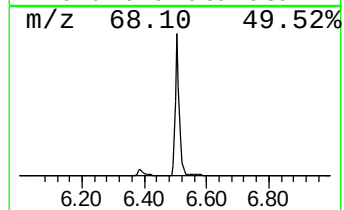
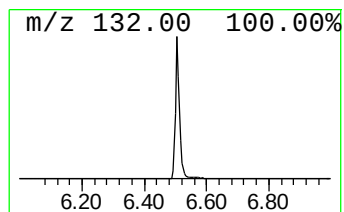
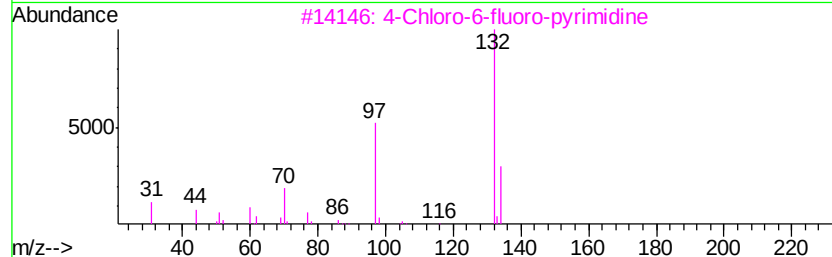
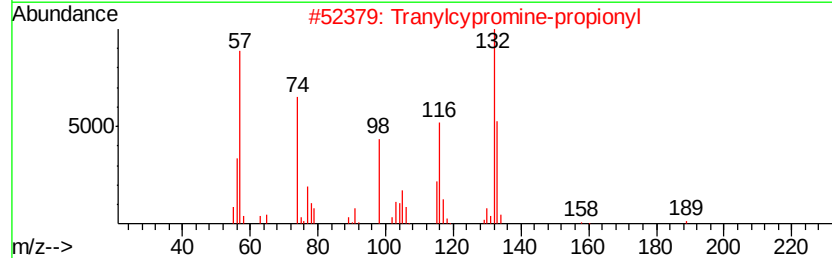
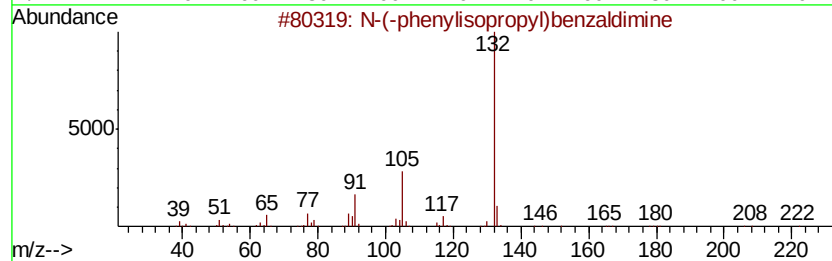
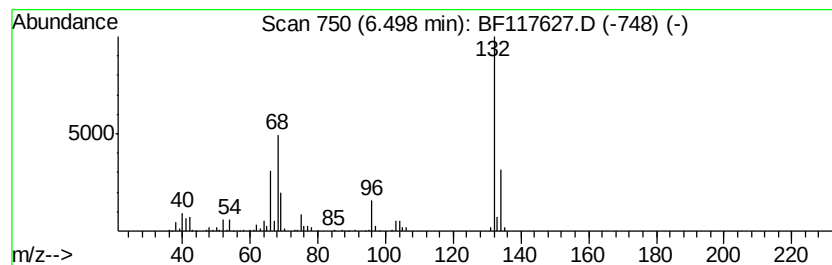
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	80.65 ng	846377	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-(-phenylisopropyl)benzalimine	223	C16H17N	1000379-01-3	10
2		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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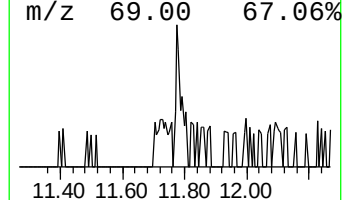
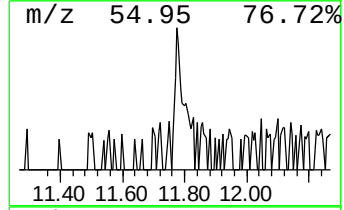
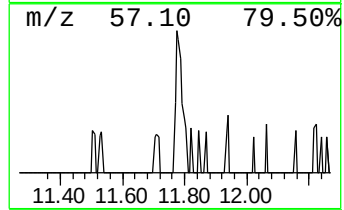
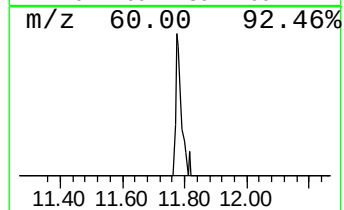
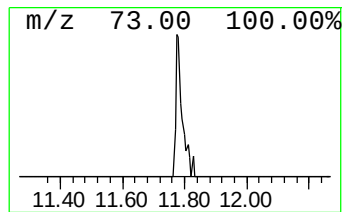
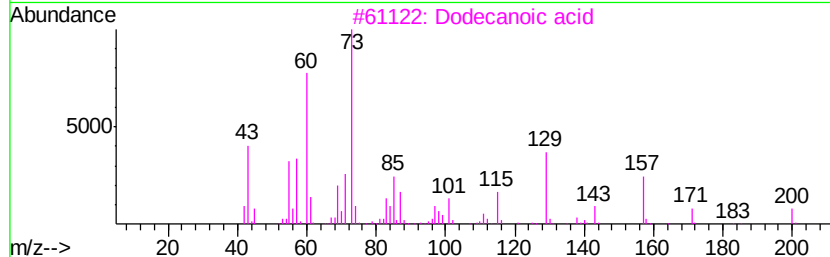
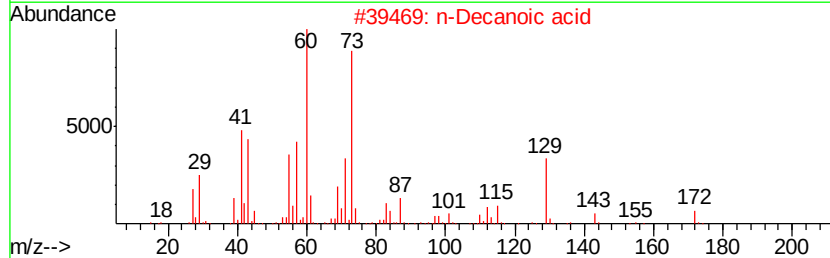
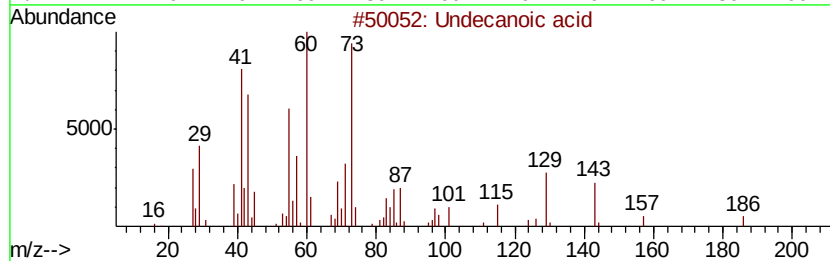
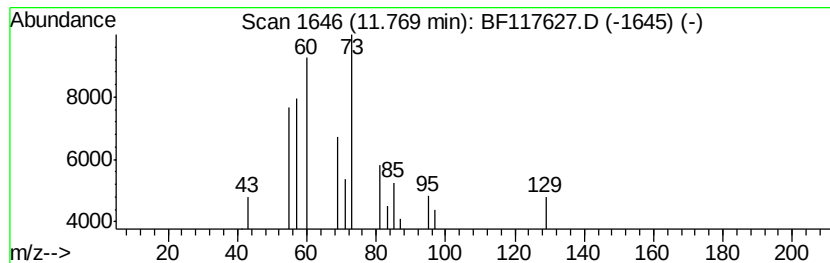
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.19 ng	24957	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid		186	C11H22O2	000112-37-8	64
2	n-Decanoic acid		172	C10H20O2	000334-48-5	59
3	Dodecanoic acid		200	C12H24O2	000143-07-7	50
4	.alpha.-D-Glucopyranose, 4-O-.be...		342	C12H22O11	014641-93-1	50
5	Decanoic acid, silver(1+) salt		278	C10H19AgO2	013126-67-5	47



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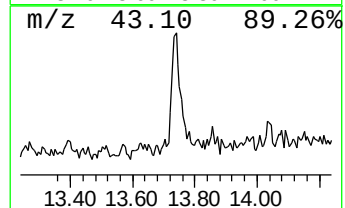
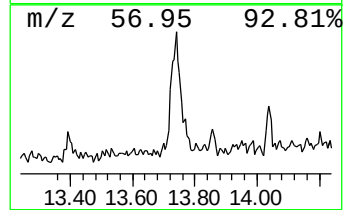
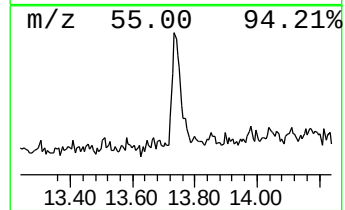
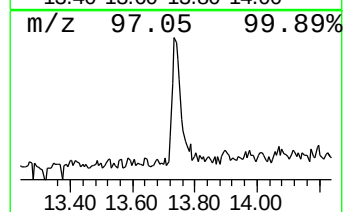
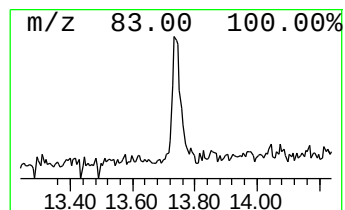
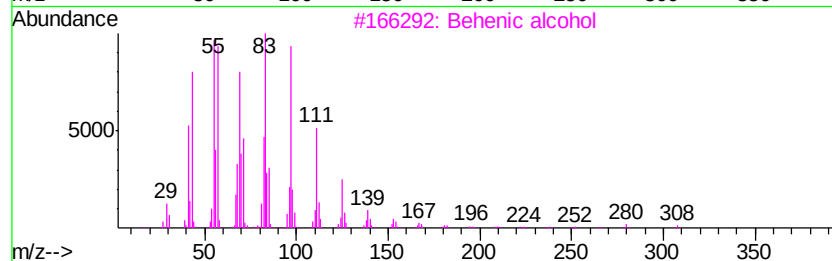
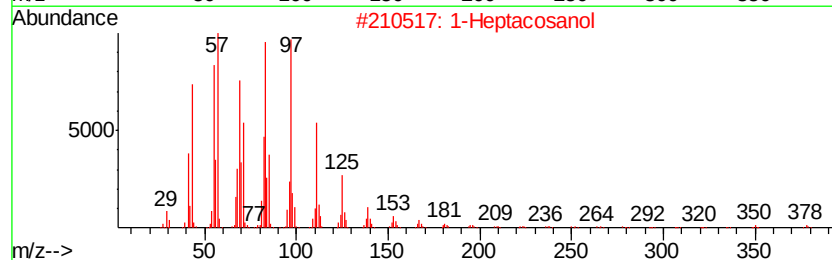
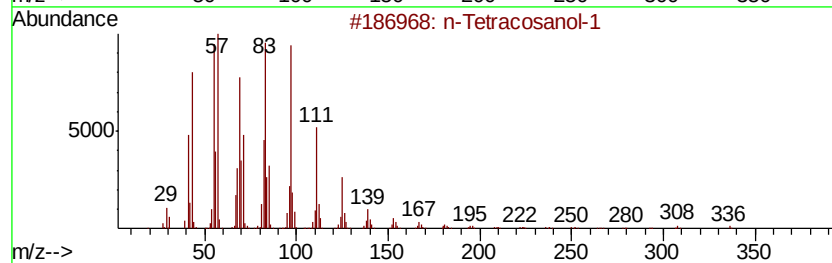
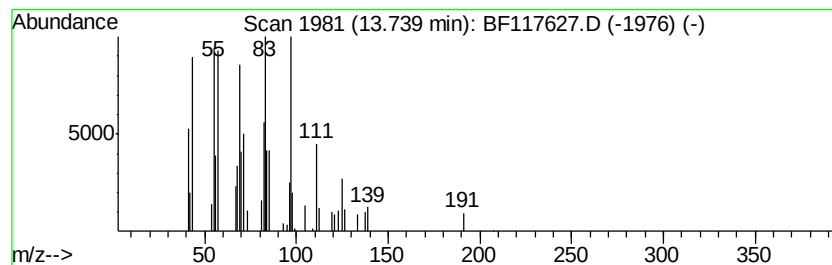
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.74	6.37 ng	85700	Chrysene-d12		13.90
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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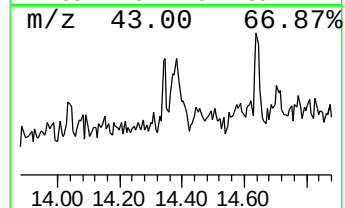
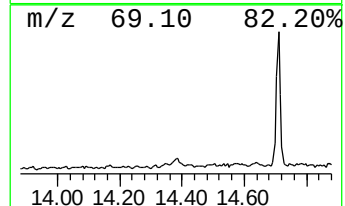
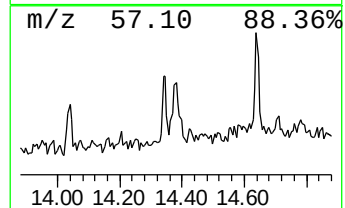
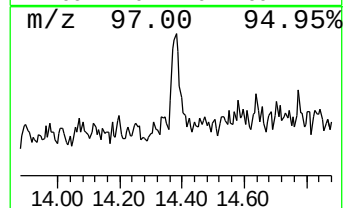
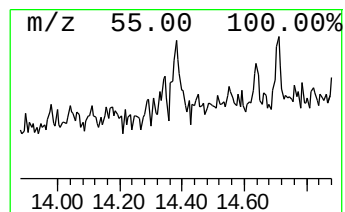
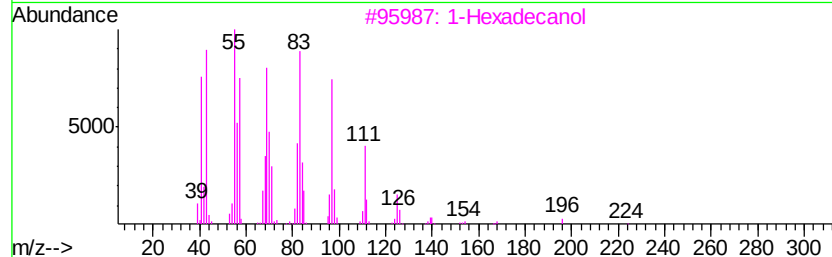
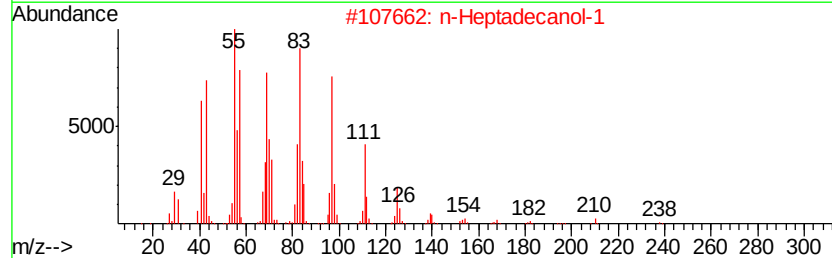
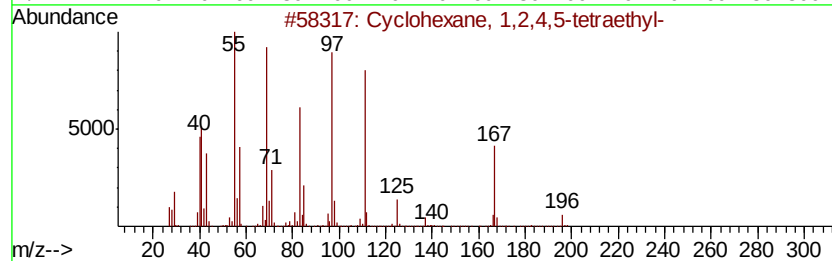
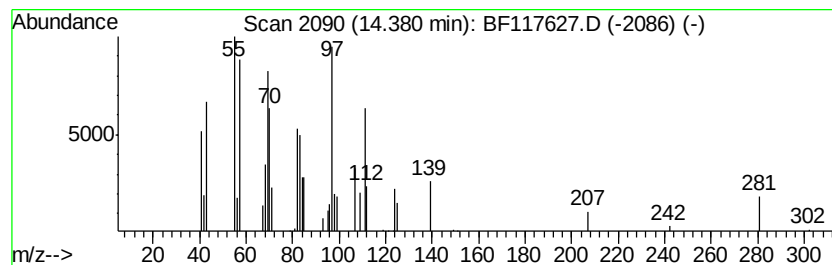
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexane, 1,2,4,5-tetrae... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	2.07 ng	27841	Chrysene-d12	13.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,2,4,5-tetraethyl-	196	C14H28	061142-00-5	50
2		n-Heptadecanol-1	256	C17H36O	001454-85-9	47
3		1-Hexadecanol	242	C16H34O	036653-82-4	47
4		Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	43
5		Heptanedioic acid, 4-methyl-, di...	202	C10H18O4	004751-49-9	43



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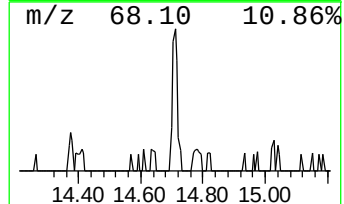
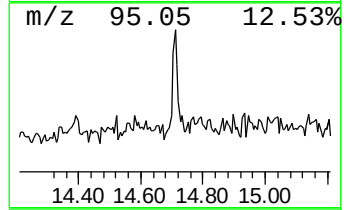
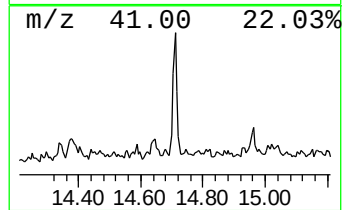
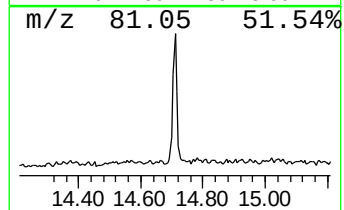
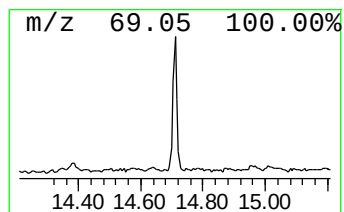
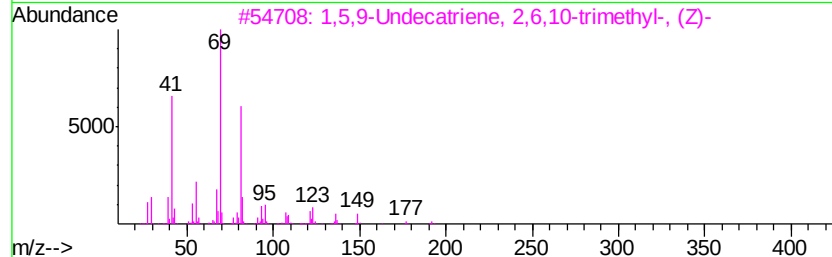
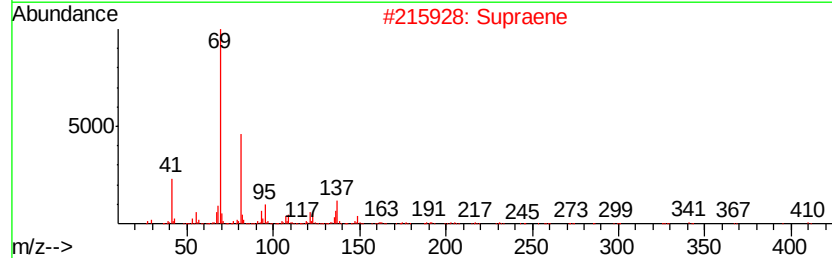
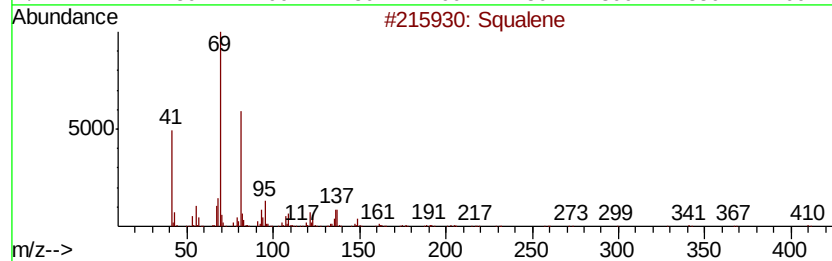
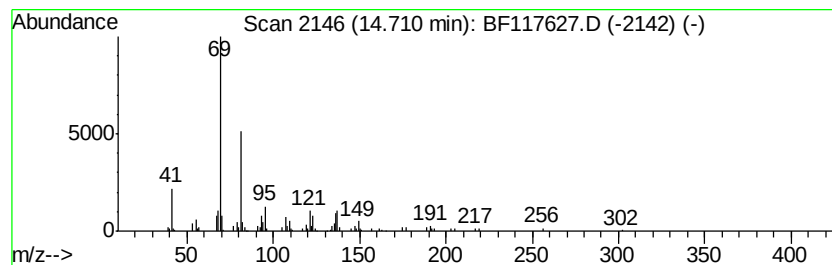
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Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	8.26 ng	84100	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
4		3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	83
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	80



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
154-24-(0-2)

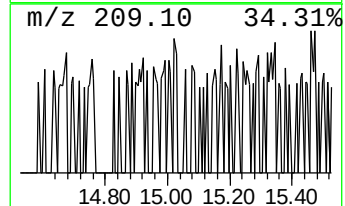
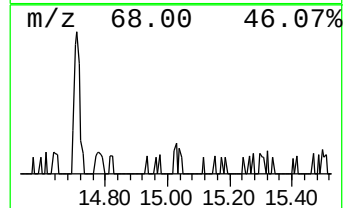
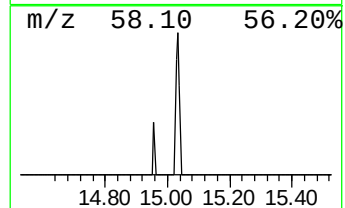
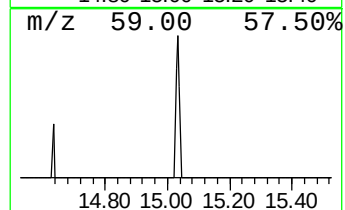
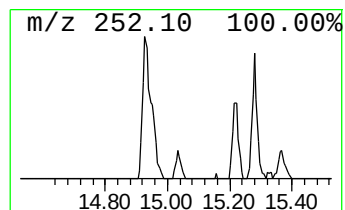
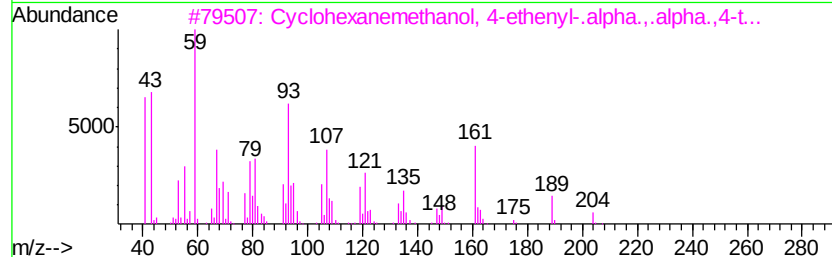
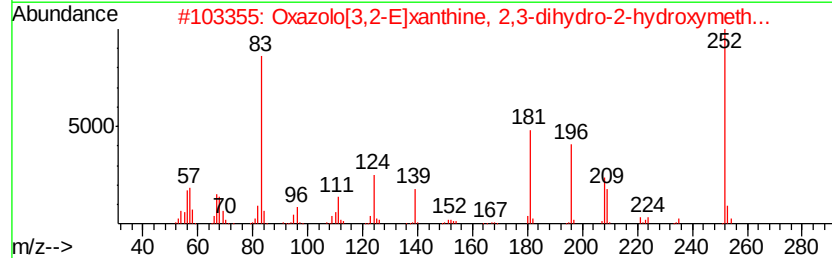
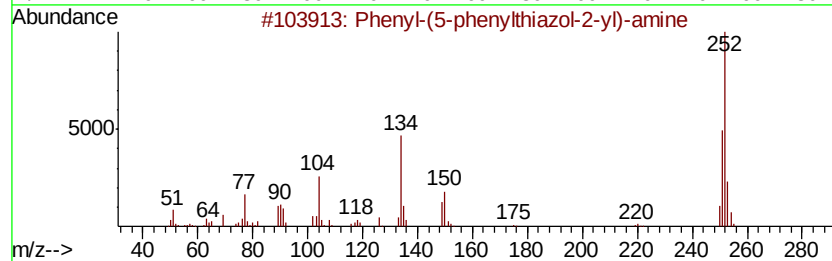
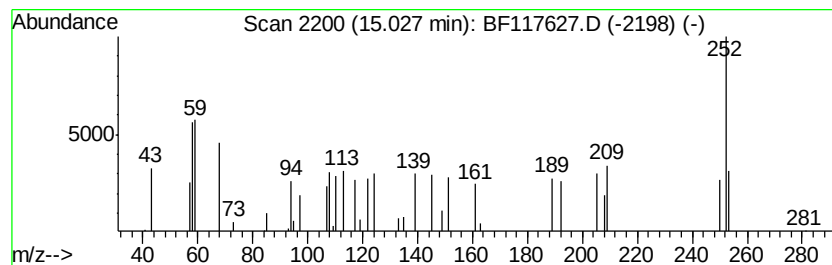
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.03 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	2.62 ng	26663	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenyl-(5-phenylthiazol-2-yl)-amine	252	C15H12N2S	306321-46-0	12
2		Oxazolo[3,2-E]xanthine, 2,3-dihy...	252	C10H12N4O4	1000285-58-3	12
3		Cyclohexanemethanol, 4-ethenyl-....	222	C15H26O	000639-99-6	10
4		N-(3-Nitro-thiobenzoyl)-morpholine	252	C11H12N2O3S	050903-05-4	9
5		Naphthalene, 1-chloro-2,4-dinitro-	252	C10H5ClN2O4	002401-85-6	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117627.D
Acq On : 30 Oct 2019 16:25
Operator : JU
Sample : K5541-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

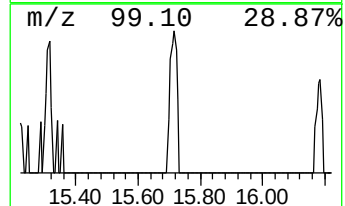
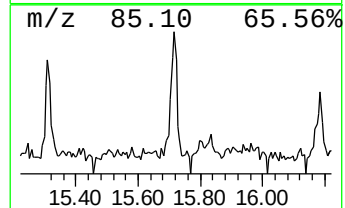
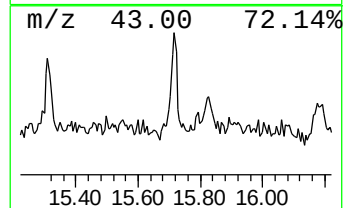
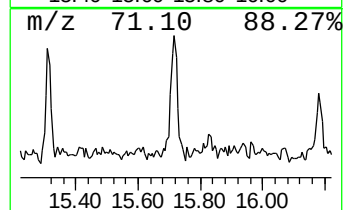
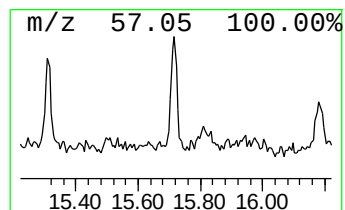
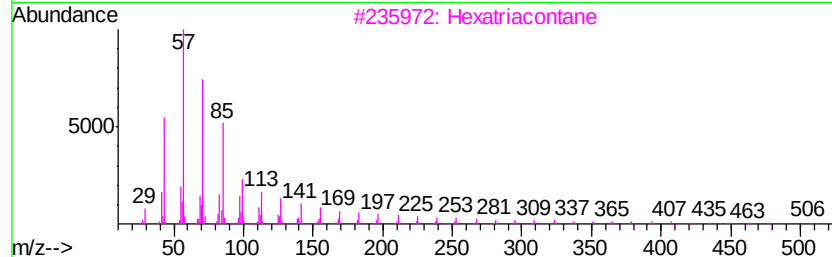
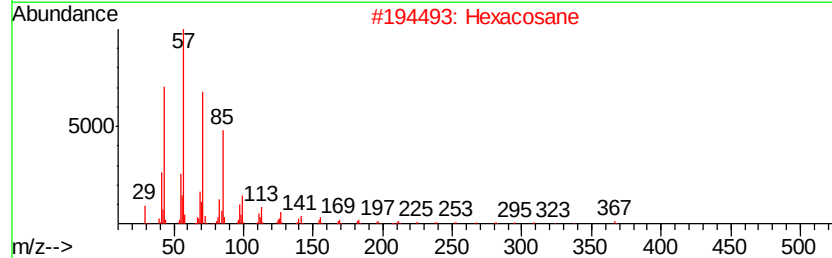
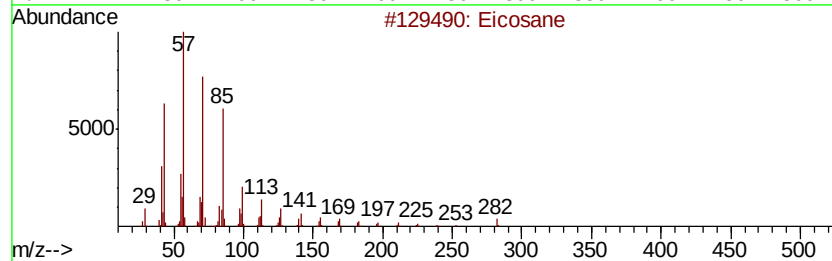
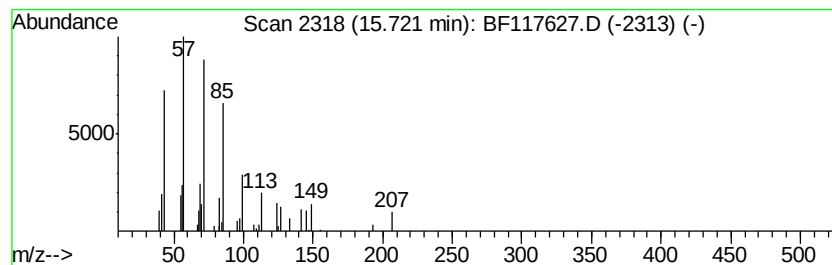
Instrument :
BNA_F
ClientSampleId :
154-24-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.43 ng	34904	Perylene-d12	15.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	87
2	Hexacosane	366 C26H54	000630-01-3	64
3	Hexatriacontane	507 C36H74	000630-06-8	64
4	Tetratetracontane	619 C44H90	007098-22-8	64
5	Docosane, 2,21-dimethyl-	338 C24H50	077536-31-3	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
Data File : BF117627.D
Acq On : 30 Oct 2019 16:25
Operator : JU
Sample : K5541-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
154-24-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.50	6.50	80.7	ng	846377	1	6.73	209880	20.0
Undecanoic acid	11.77	2.2	ng	24957	4	11.25	228208	20.0
n-Tetracosanol-1	13.74	6.4	ng	85700	5	13.90	268873	20.0
Cyclohexane, 1,2,...	14.38	2.1	ng	27841	5	13.90	268873	20.0
Squalene	14.71	8.3	ng	84100	6	15.33	203577	20.0
unknown15.03	15.03	2.6	ng	26663	6	15.33	203577	20.0
Eicosane	15.72	3.4	ng	34904	6	15.33	203577	20.0