

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
 Data File : BF117492.D
 Acq On : 23 Oct 2019 19:24
 Operator : JU
 Sample : K5139-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-03-102119

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	5.351	552	555	582	rBV	854674	929606	86.65%	8.876%
2	6.381	726	730	744	rBV	1033537	1041094	97.04%	9.940%
3	6.504	747	751	762	rVB	1227211	1058617	98.67%	10.108%
4	6.734	787	790	801	rBV	247587	248072	23.12%	2.369%
5	6.887	812	816	825	rBV	900646	763911	71.20%	7.294%
6	7.298	882	886	902	rBV	593120	619710	57.76%	5.917%
7	8.010	1004	1007	1020	rBV	326808	322960	30.10%	3.084%
8	9.086	1186	1190	1193	rBV	1309673	1072881	100.00%	10.244%
9	9.480	1254	1257	1272	rBB	118695	101441	9.46%	0.969%
10	9.763	1301	1305	1318	rBV	454035	389778	36.33%	3.722%
11	10.551	1436	1439	1455	rBV	689316	670645	62.51%	6.403%
12	11.245	1554	1557	1561	rBV	380022	360744	33.62%	3.444%
13	11.774	1645	1647	1655	rBV2	46856	49162	4.58%	0.469%
14	12.463	1761	1764	1768	rBV	39880	39996	3.73%	0.382%
15	12.557	1777	1780	1788	rBV3	11055	16105	1.50%	0.154%
16	12.692	1798	1803	1811	rBV	41816	48606	4.53%	0.464%
17	12.827	1822	1826	1830	rBV	1062452	994333	92.68%	9.494%
18	13.398	1919	1923	1926	rBV3	17162	14107	1.31%	0.135%
19	13.727	1976	1979	1992	rVB2	60323	93755	8.74%	0.895%
20	13.886	2003	2006	2020	rVB	241798	296215	27.61%	2.828%
21	14.045	2029	2033	2036	rBV	102586	95088	8.86%	0.908%
22	14.286	2068	2074	2076	rBV5	7631	12842	1.20%	0.123%
23	14.345	2081	2084	2088	rVV	159197	141897	13.23%	1.355%
24	14.645	2131	2135	2138	rBV	189697	178133	16.60%	1.701%
25	14.921	2178	2182	2184	rBV	17730	24960	2.33%	0.238%
26	14.957	2184	2188	2193	rVB	169895	193259	18.01%	1.845%
27	15.204	2228	2230	2235	rVB	12595	14223	1.33%	0.136%
28	15.268	2237	2241	2244	rBV	16595	18400	1.72%	0.176%
29	15.315	2244	2249	2259	rVB2	317517	415124	38.69%	3.964%
30	15.721	2312	2318	2322	rBV	86044	120237	11.21%	1.148%
31	16.186	2392	2397	2403	rBV2	43942	71845	6.70%	0.686%
32	16.739	2485	2491	2497	rVB9	19503	37491	3.49%	0.358%
33	16.892	2511	2517	2521	rBV8	8050	18131	1.69%	0.173%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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

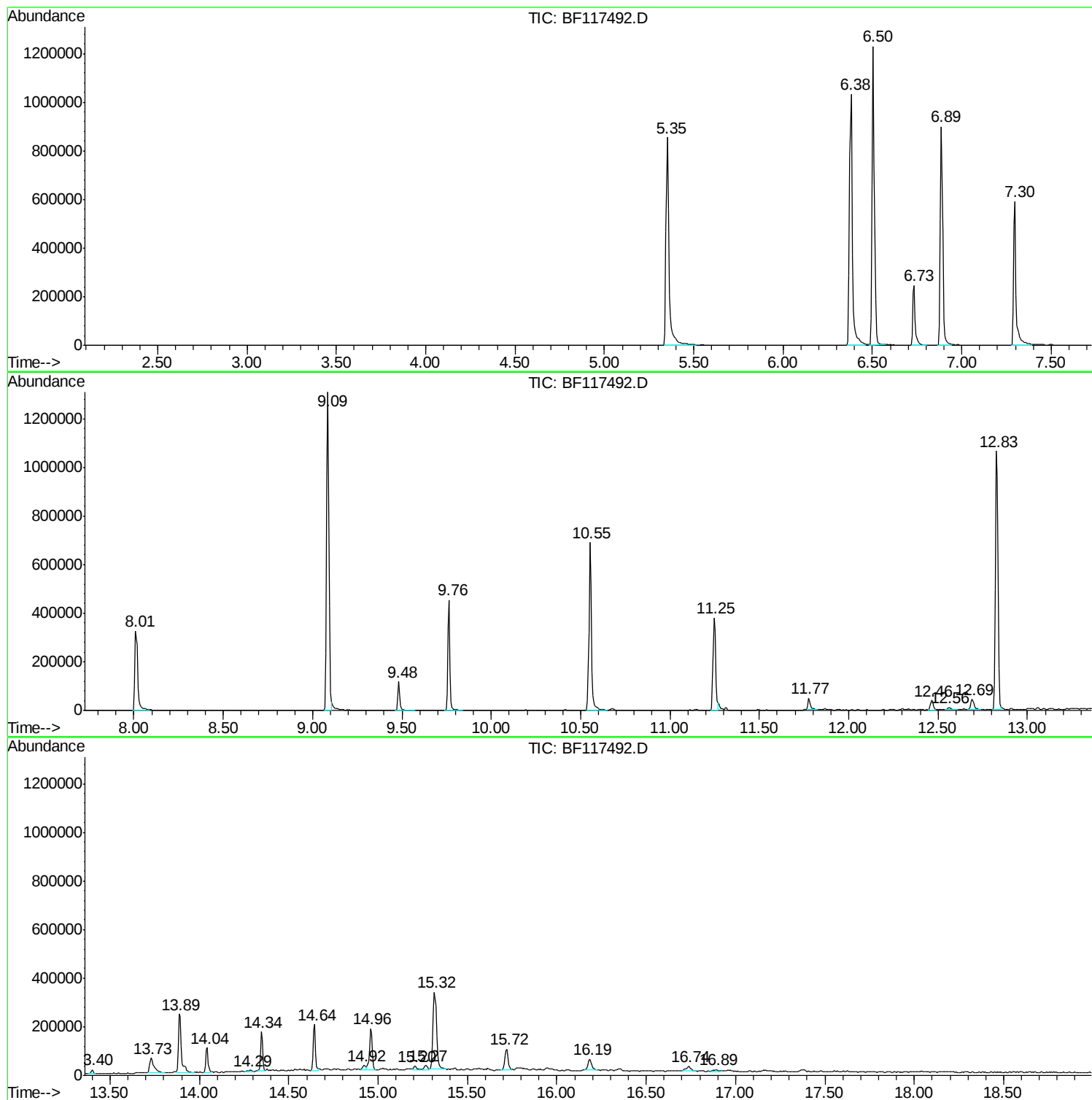
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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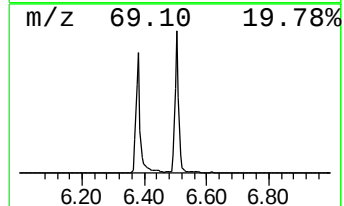
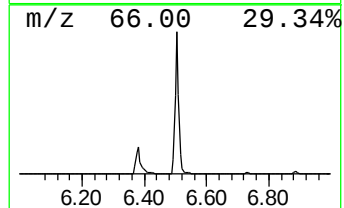
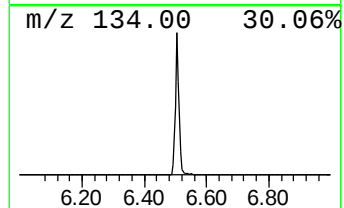
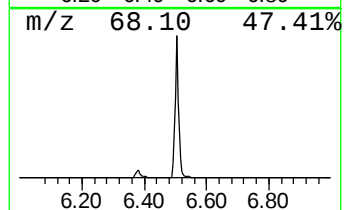
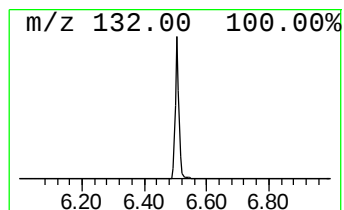
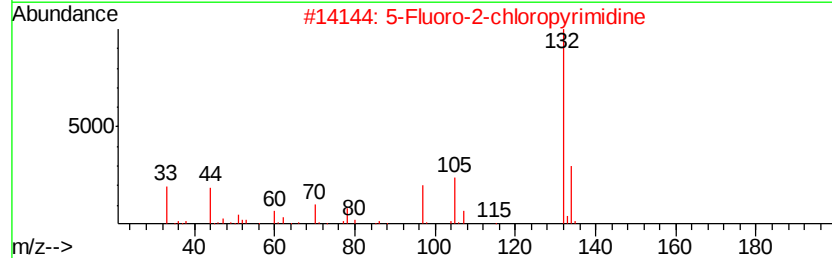
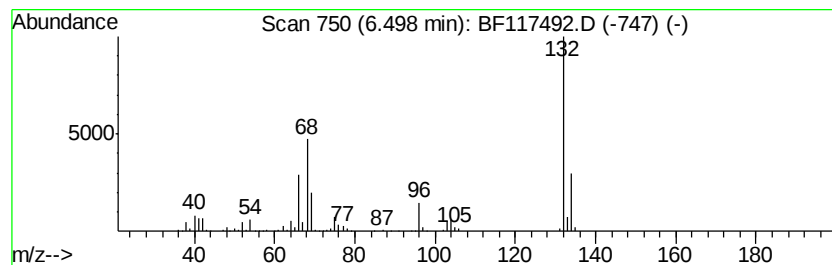
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	85.35 ng	1058620	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Xenon	132	Xe	007440-63-3	9



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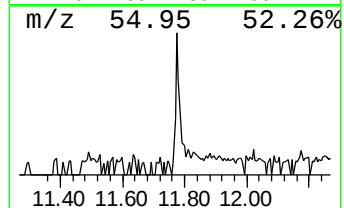
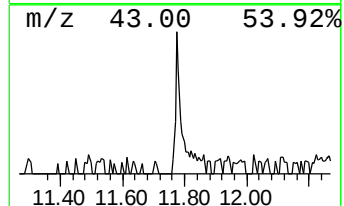
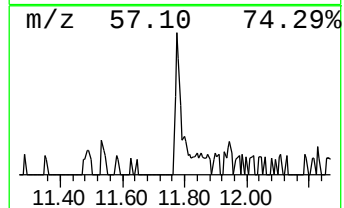
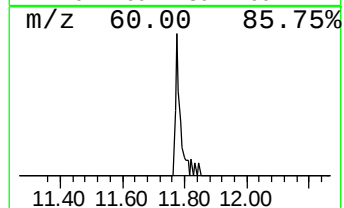
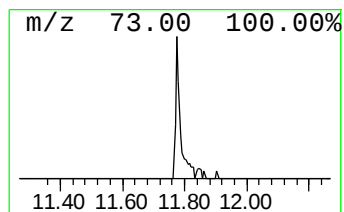
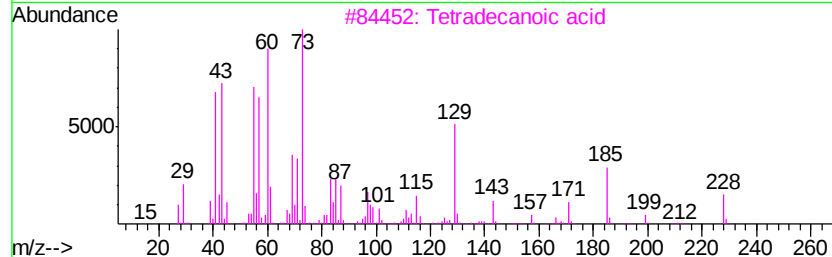
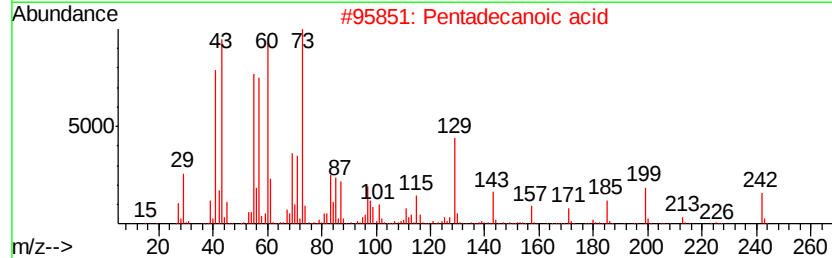
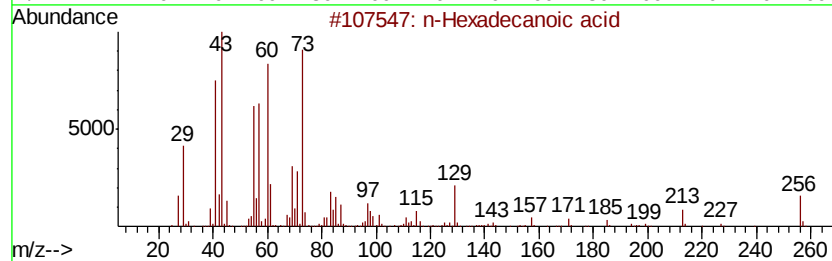
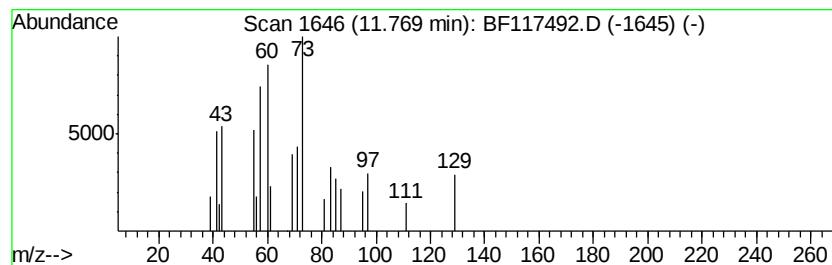
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	2.73 ng	49162	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	47



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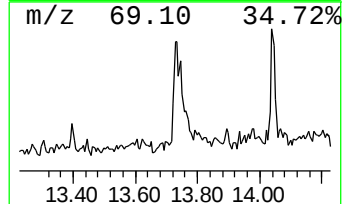
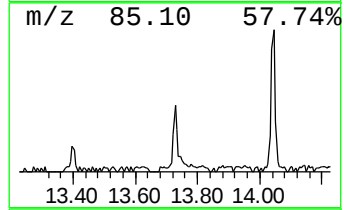
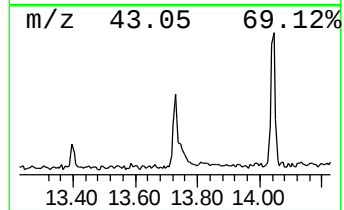
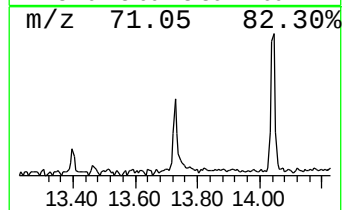
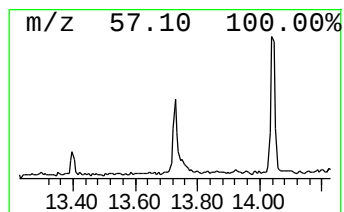
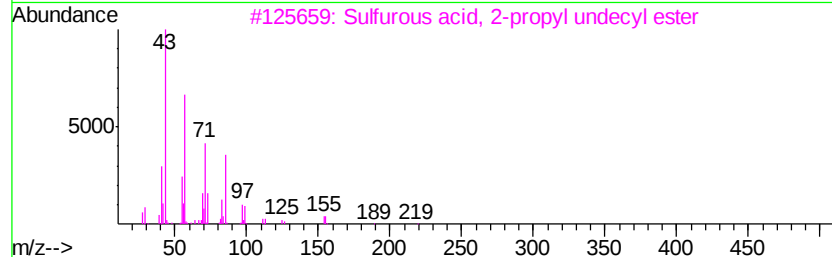
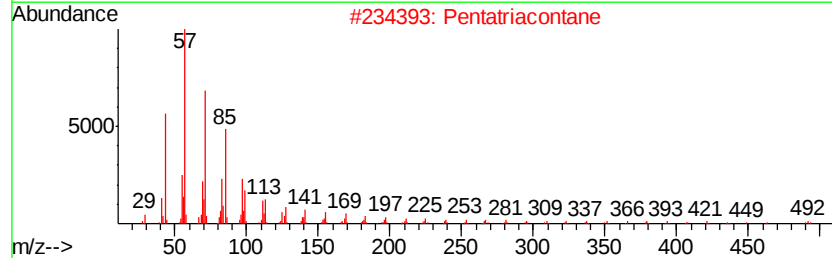
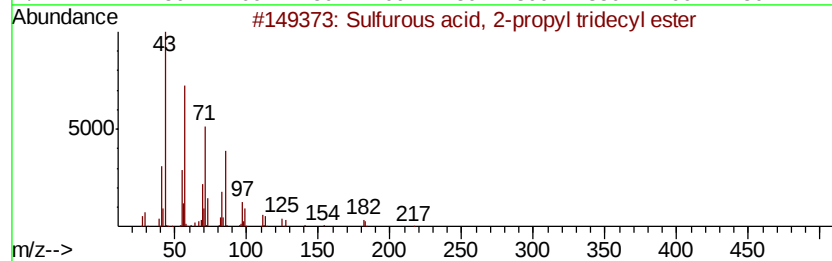
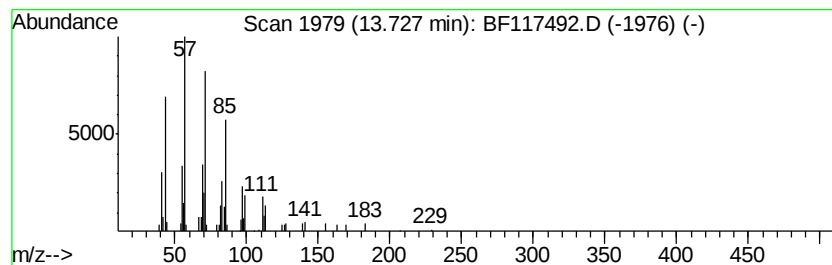
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Sulfurous acid, 2-propyl tr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.33 ng	93755	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-propyl tridecyl...	306	C16H34O3S	1000309-12-4	90
2		Pentatriacontane	493	C35H72	000630-07-9	86
3		Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	80
4		Heneicosane	296	C21H44	000629-94-7	72
5		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	72



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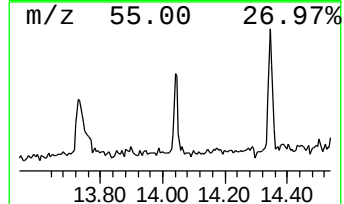
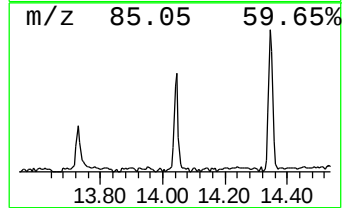
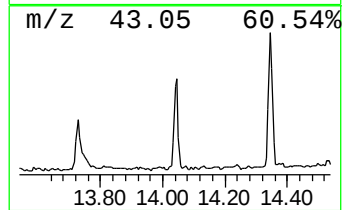
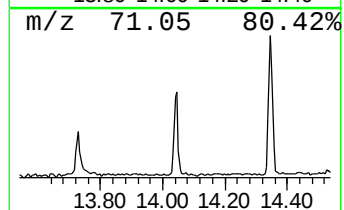
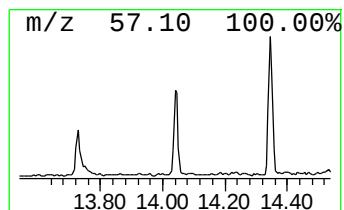
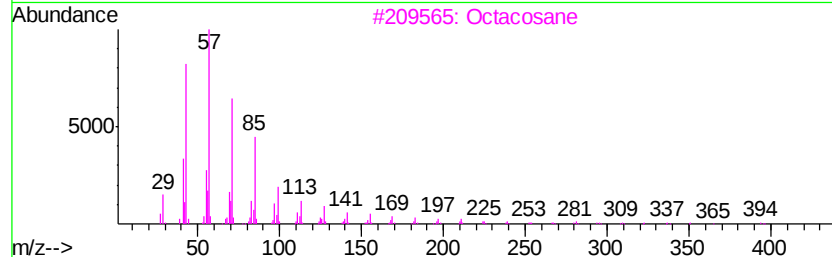
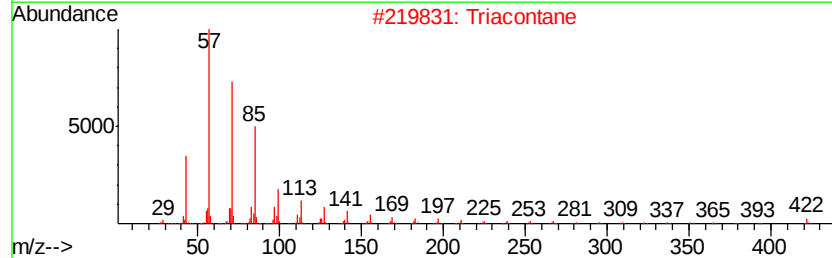
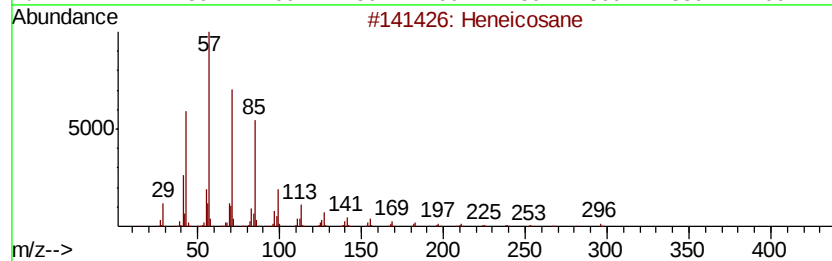
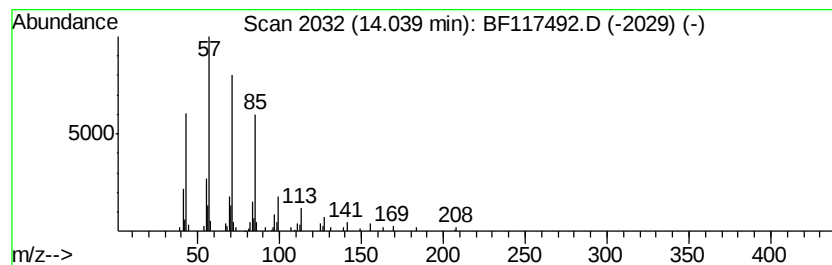
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	6.42 ng	95088	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Triacotane		422	C30H62	000638-68-6	90
3	Octacosane		394	C28H58	000630-02-4	90
4	2-methyloctacosane		408	C29H60	1000376-72-8	90
5	Heptadecane		240	C17H36	000629-78-7	90



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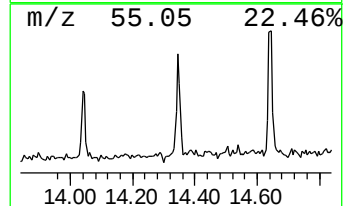
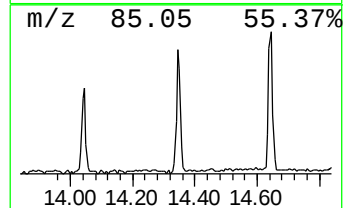
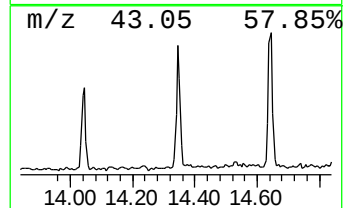
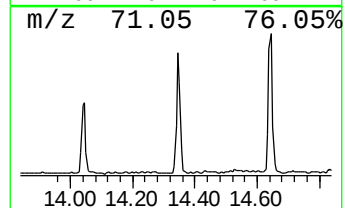
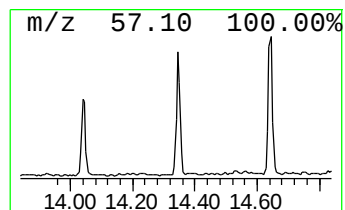
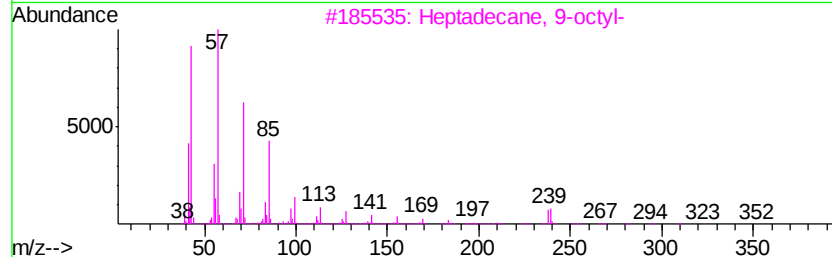
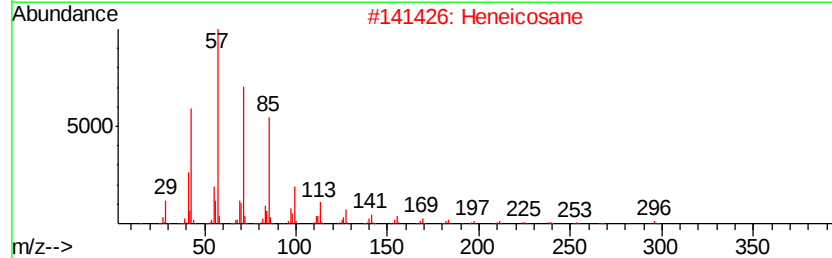
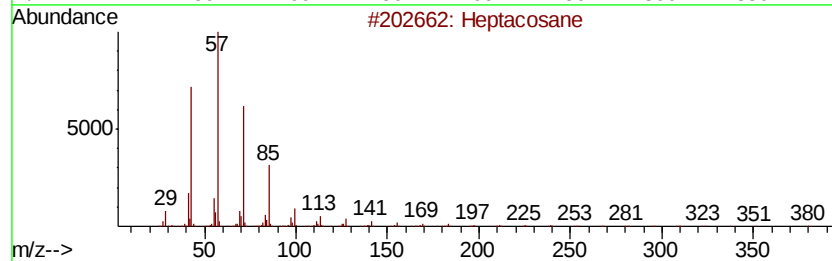
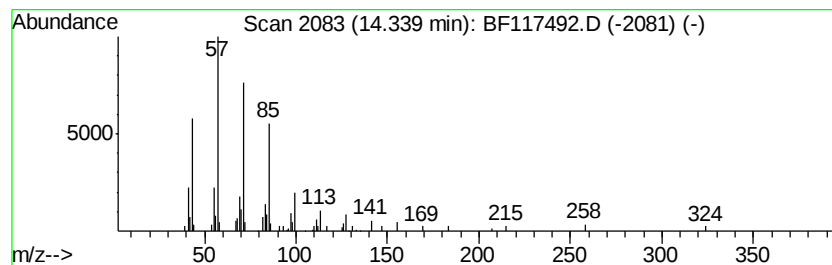
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	9.58 ng	141897	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Hexacosane		366	C26H54	000630-01-3	91
5	Octadecane		254	C18H38	000593-45-3	91



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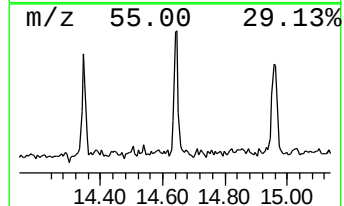
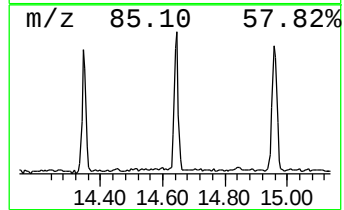
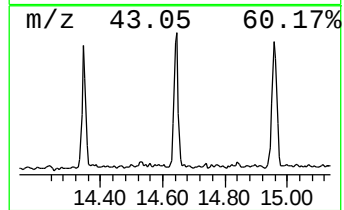
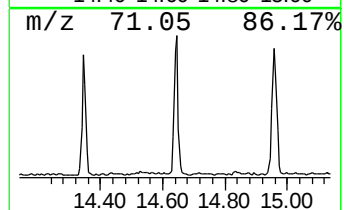
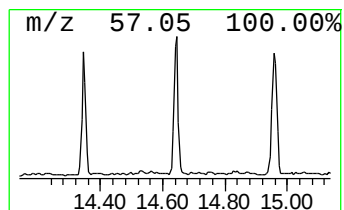
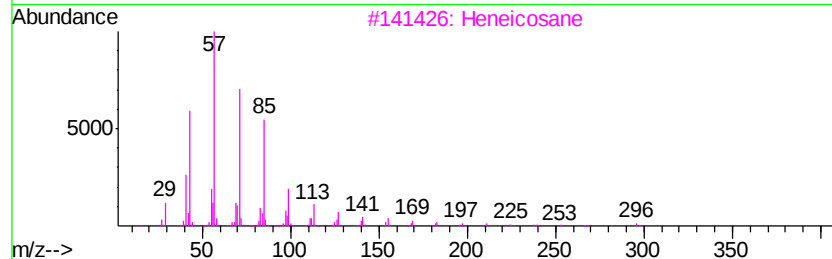
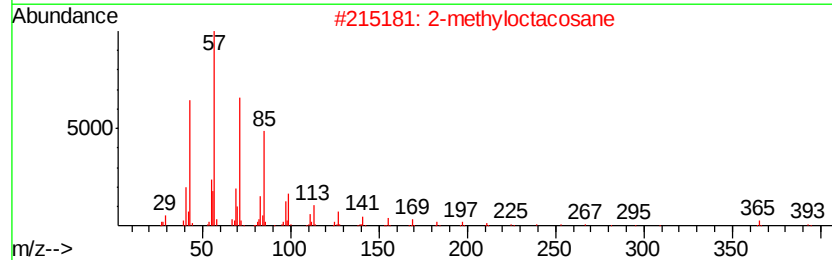
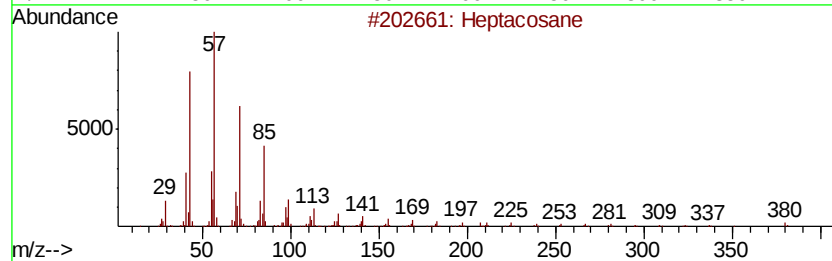
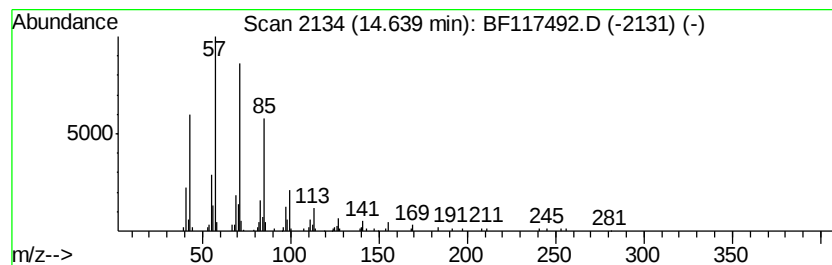
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	8.58 ng	178133	Perylene-d12	15.32

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
 Data File : BF117492.D
 Acq On : 23 Oct 2019 19:24
 Operator : JU
 Sample : K5139-01
 Misc :
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Instrument :
 BNA_F
 ClientSampleId :
 BU-03-102119

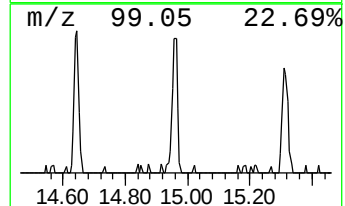
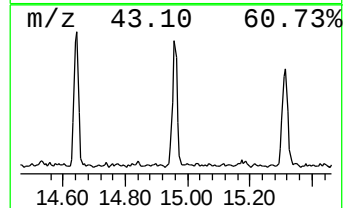
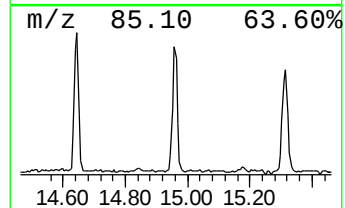
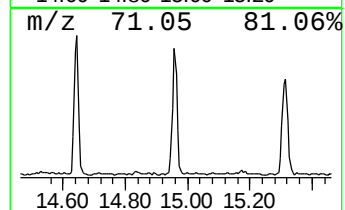
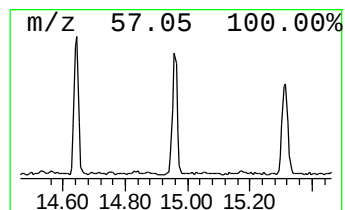
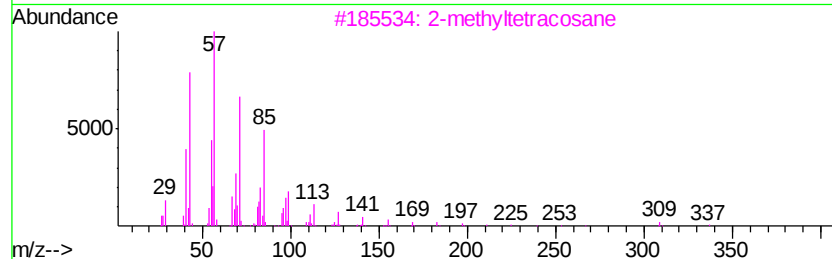
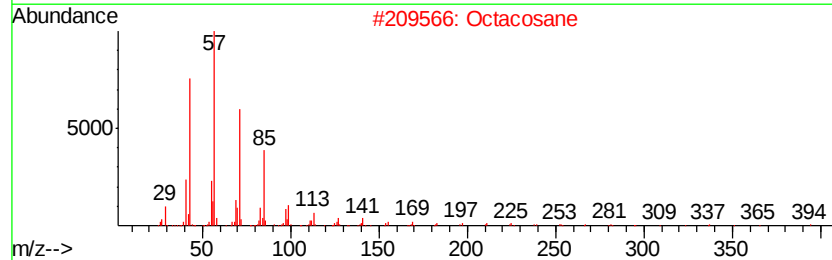
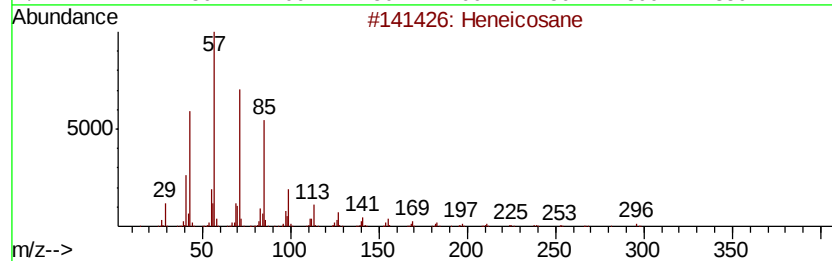
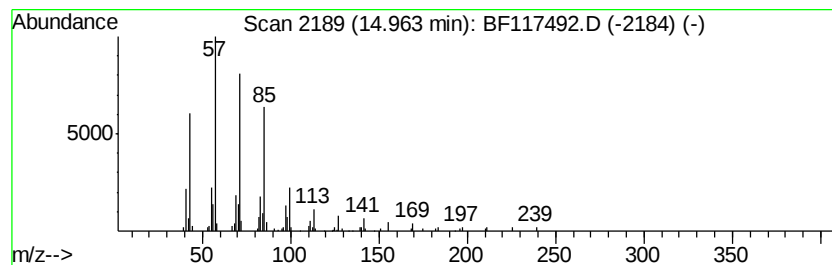
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	9.31 ng	193259	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	90
3		2-methyltetracosane	352	C25H52	1000376-72-6	90
4		triacontane	422	C30H62	000638-68-6	90
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117492.D
Acq On : 23 Oct 2019 19:24
Operator : JU
Sample : K5139-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-102119

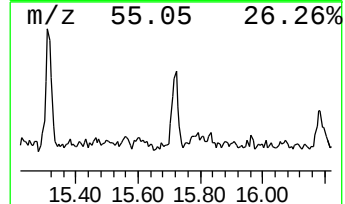
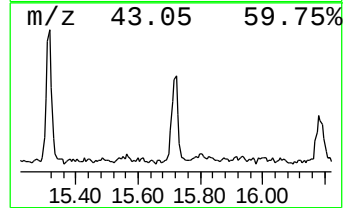
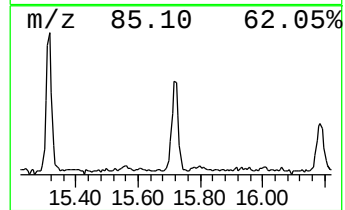
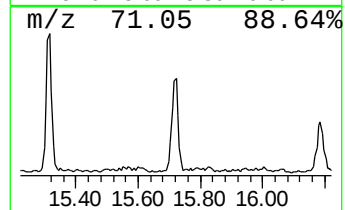
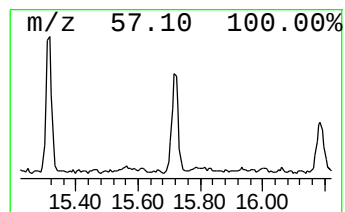
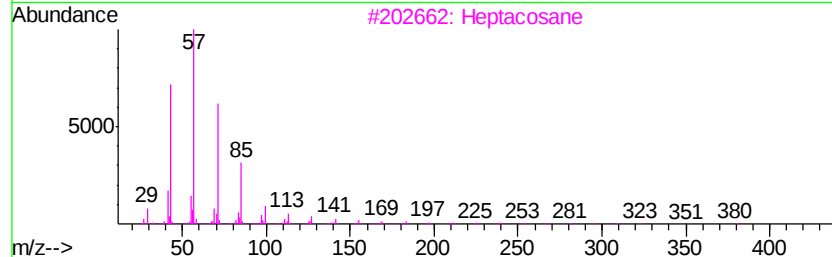
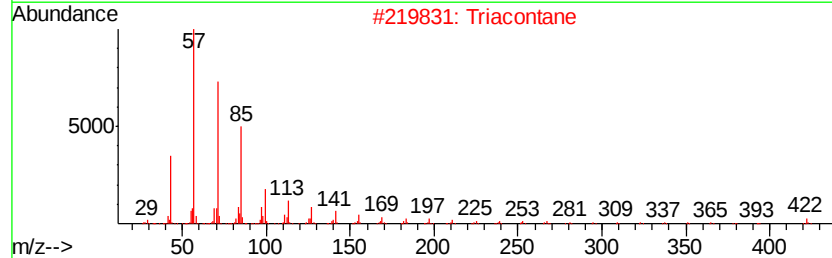
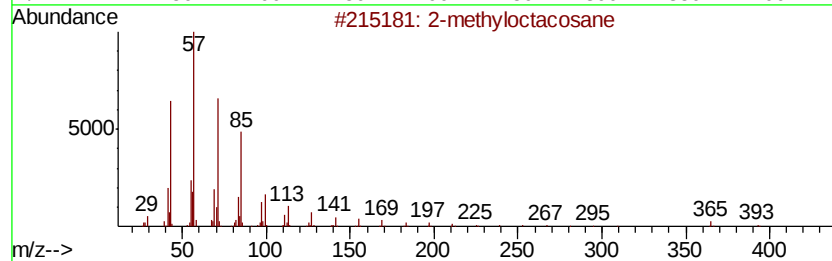
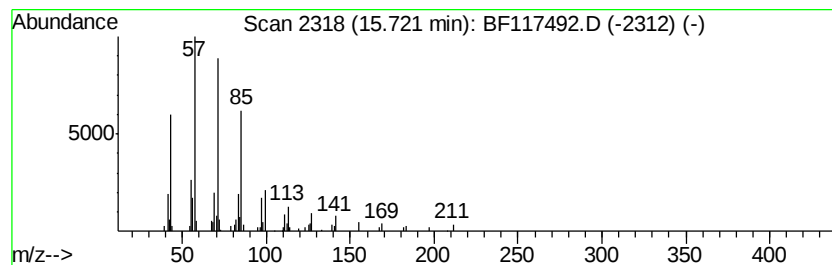
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	5.79 ng	120237	Perylene-d12	15.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane		408	C29H60	1000376-72-8	91
2	Triacontane		422	C30H62	000638-68-6	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	2-methyltetracosane		352	C25H52	1000376-72-6	90
5	Tetratetracontane		619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102319\
Data File : BF117492.D
Acq On : 23 Oct 2019 19:24
Operator : JU
Sample : K5139-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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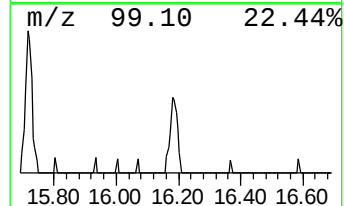
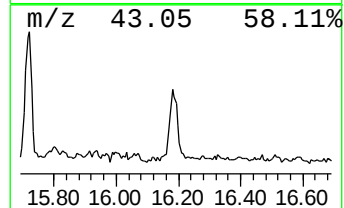
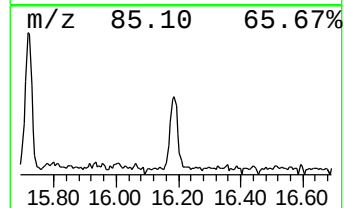
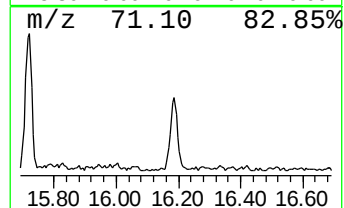
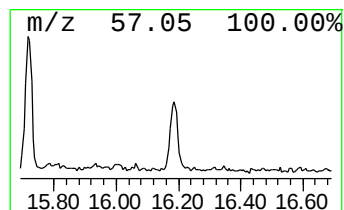
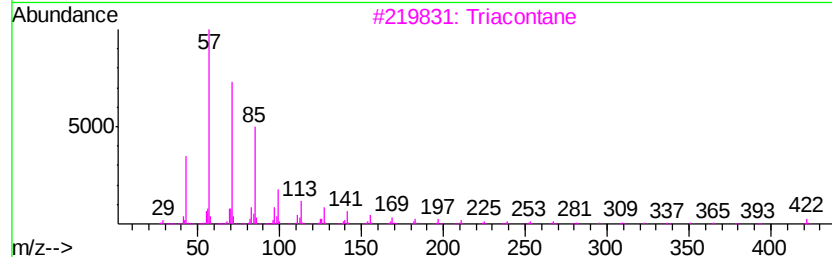
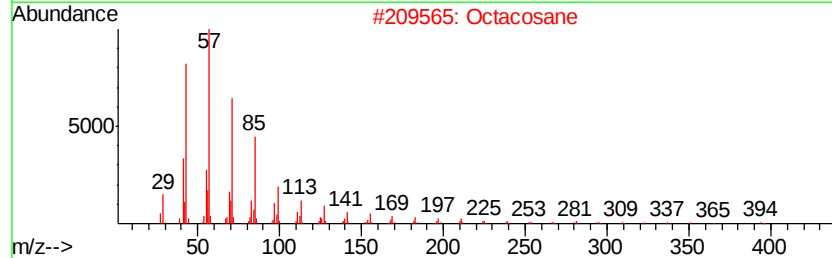
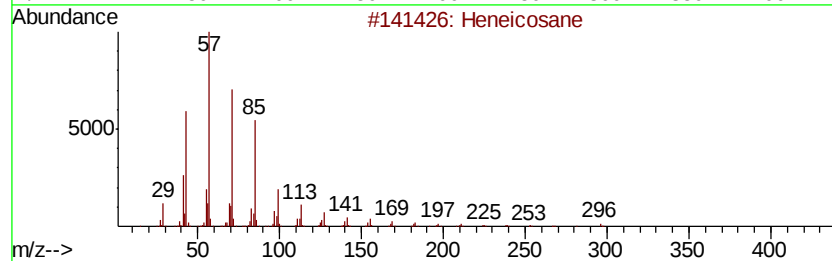
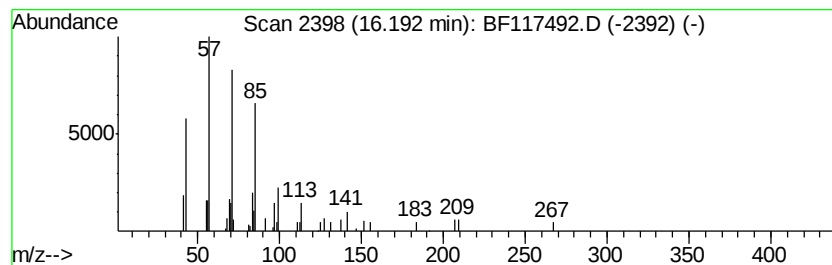
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	3.46 ng	71845	Perylene-d12	15.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Triacosane	422	C30H62	000638-68-6	91
4			Hentriacontane	437	C31H64	000630-04-6	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102319\
Data File : BF117492.D
Acq On : 23 Oct 2019 19:24
Operator : JU
Sample : K5139-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-03-102119

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	85.3	ng	1058620	1	6.73	248072	20.0
n-Hexadecanoic acid	11.77	2.7	ng	49162	4	11.25	360744	20.0
Sulfurous acid, 2...	13.73	6.3	ng	93755	5	13.89	296215	20.0
Heneicosane	14.04	6.4	ng	95088	5	13.89	296215	20.0
Heptacosane	14.34	9.6	ng	141897	5	13.89	296215	20.0
2-methyloctacosane	14.64	8.6	ng	178133	6	15.32	415124	20.0
Octacosane	14.96	9.3	ng	193259	6	15.32	415124	20.0
triacontane	15.72	5.8	ng	120237	6	15.32	415124	20.0
Hentriacontane	16.19	3.5	ng	71845	6	15.32	415124	20.0