

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051119\
 Data File : BF114157.D
 Acq On : 11 May 2019 15:21
 Operator : JU/SJ
 Sample : K2763-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P021-SS005-0206-01

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-BF051019.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	5.063	502	506	517	rVB	243831	289039	4.98%	0.512%
2	5.475	571	576	579	rBV	5488235	5036878	86.77%	8.924%
3	6.487	743	748	751	rBV	5959386	5715866	98.46%	10.127%
4	6.622	767	771	774	rBV	6151410	5456349	93.99%	9.667%
5	6.851	806	810	813	rBV	1875954	1596237	27.50%	2.828%
6	7.004	832	836	840	rBV	4365386	3948669	68.02%	6.996%
7	7.410	900	905	908	rBV	3999104	3606589	62.13%	6.390%
8	8.128	1023	1027	1031	rBV	2423591	2041116	35.16%	3.616%
9	9.204	1206	1210	1213	rBV	6842194	5805038	100.00%	10.285%
10	9.592	1273	1276	1279	rBV	1138227	851338	14.67%	1.508%
11	9.881	1321	1325	1329	rBV	2538663	2264839	39.02%	4.013%
12	10.669	1455	1459	1463	rBV	4152399	3802944	65.51%	6.738%
13	11.363	1574	1577	1581	rBV	2499013	2375623	40.92%	4.209%
14	11.892	1664	1667	1679	rBV	705052	713759	12.30%	1.265%
15	12.598	1785	1787	1793	rVB2	52953	65447	1.13%	0.116%
16	12.674	1797	1800	1814	rBV	193752	239824	4.13%	0.425%
17	12.951	1842	1847	1850	rBV	5587261	5266171	90.72%	9.330%
18	13.839	1995	1998	2014	rVB	1000335	1184191	20.40%	2.098%
19	14.004	2022	2026	2029	rBV	1690930	1605570	27.66%	2.845%
20	14.169	2051	2054	2060	rBV	87488	105855	1.82%	0.188%
21	14.474	2103	2106	2115	rVB2	209095	262259	4.52%	0.465%
22	14.757	2151	2154	2156	rBV	105565	109478	1.89%	0.194%
23	14.780	2156	2158	2161	rVB	185800	161150	2.78%	0.286%
24	14.857	2167	2171	2175	rVB	128303	126277	2.18%	0.224%
25	14.921	2179	2182	2186	rVB	203000	204444	3.52%	0.362%
26	15.116	2211	2215	2218	rBV	300455	365245	6.29%	0.647%
27	15.139	2218	2219	2227	rVB	152423	201361	3.47%	0.357%
28	15.468	2270	2275	2278	rBV	1318702	1701788	29.32%	3.015%
29	15.692	2310	2313	2319	rVB3	69957	96495	1.66%	0.171%
30	15.927	2348	2353	2358	rBV	318715	477159	8.22%	0.845%
31	15.980	2358	2362	2369	rVV3	116755	240144	4.14%	0.425%
32	16.427	2433	2438	2445	rBV	132077	237634	4.09%	0.421%
33	17.021	2534	2539	2546	rVB2	83707	166867	2.87%	0.296%
34	17.274	2578	2582	2589	rVB8	64669	121095	2.09%	0.215%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

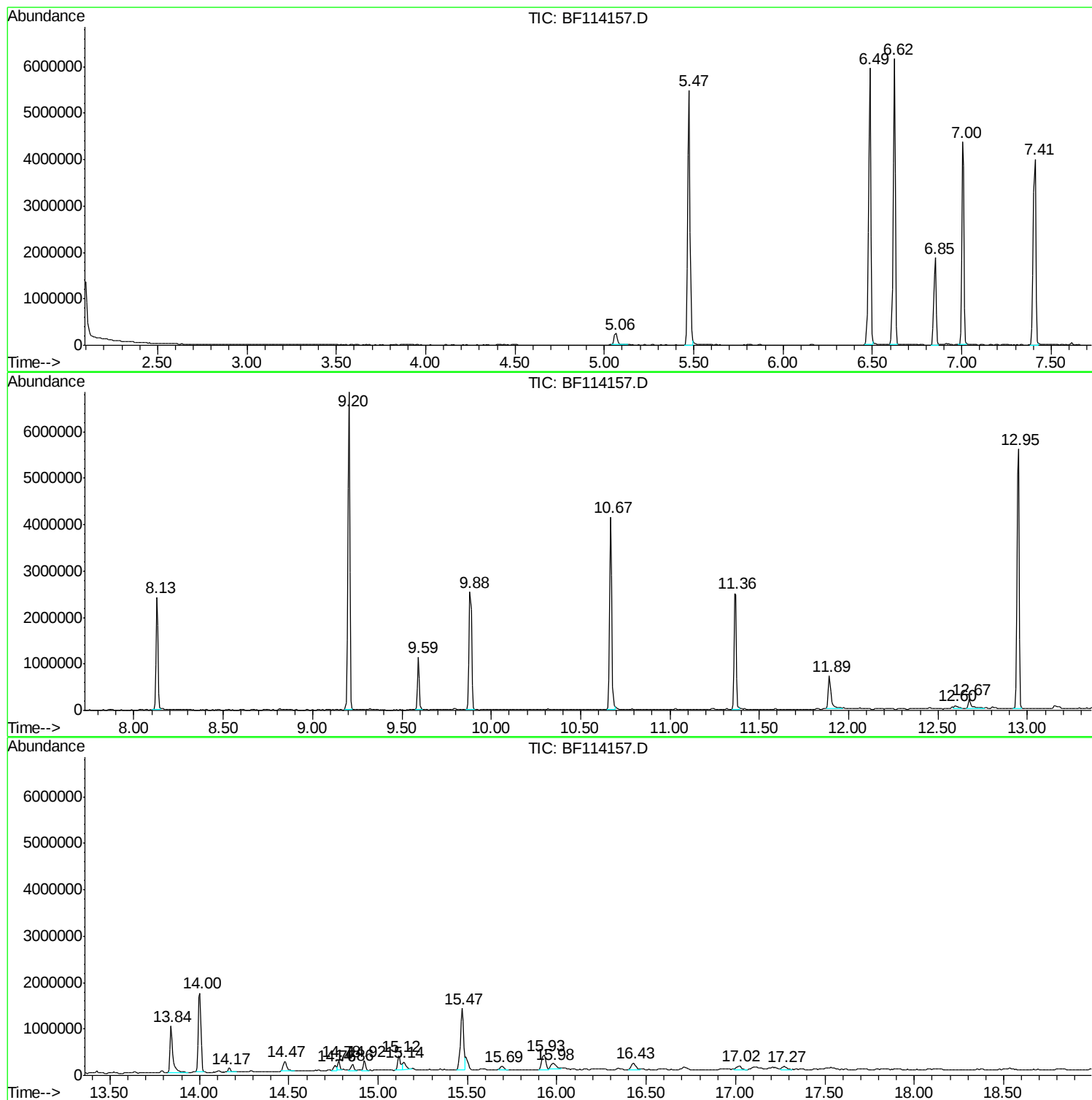
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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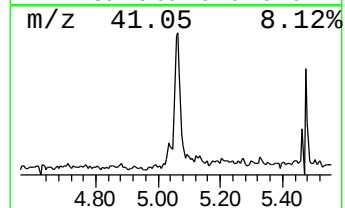
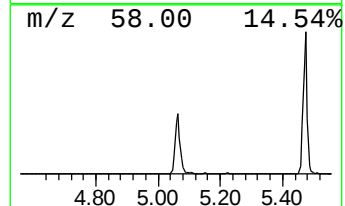
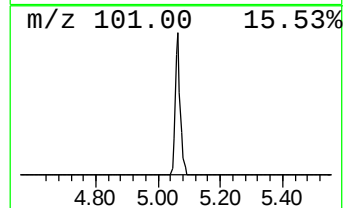
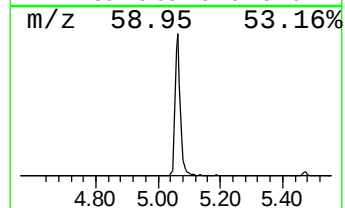
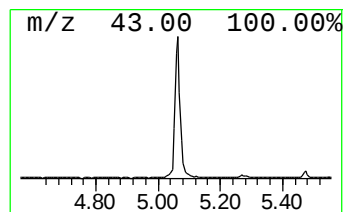
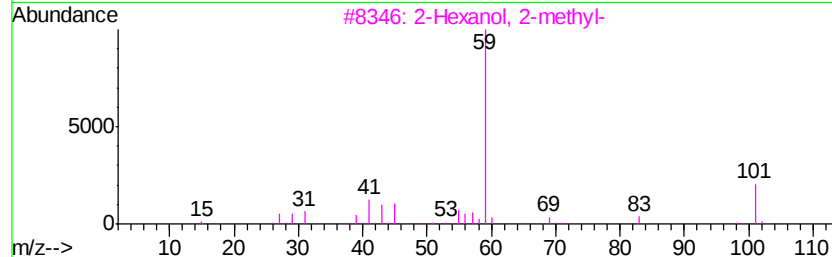
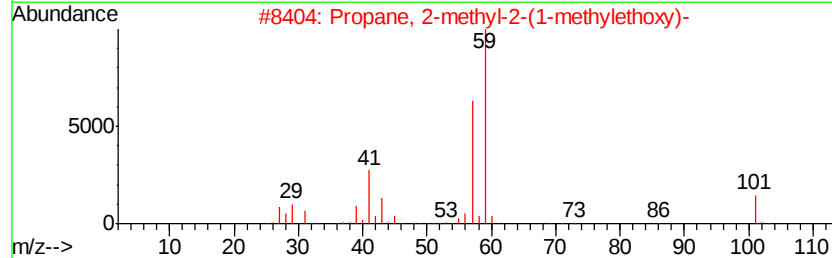
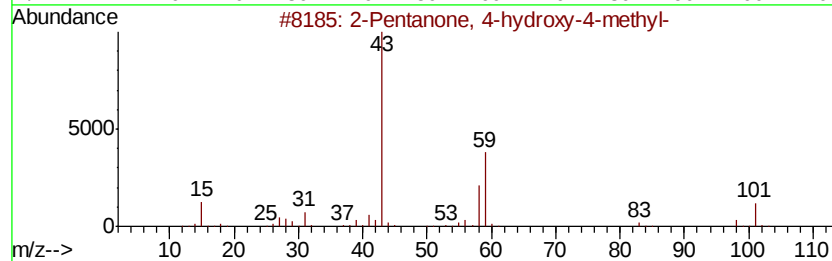
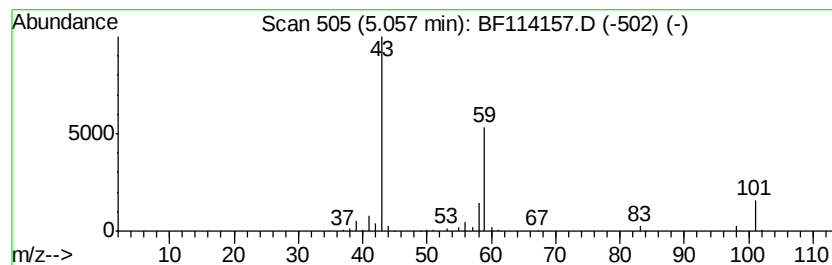
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	3.62 ng	289039	1,4-Dichlorobenzene-d4	6.85

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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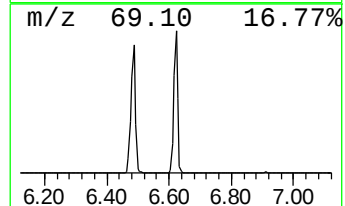
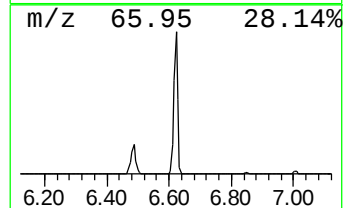
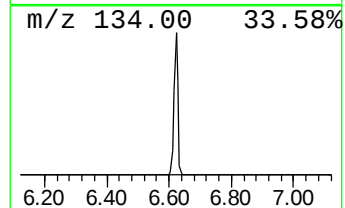
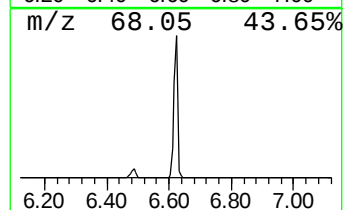
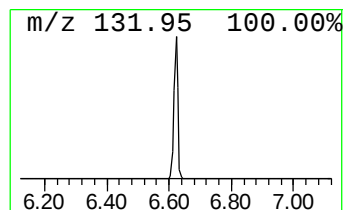
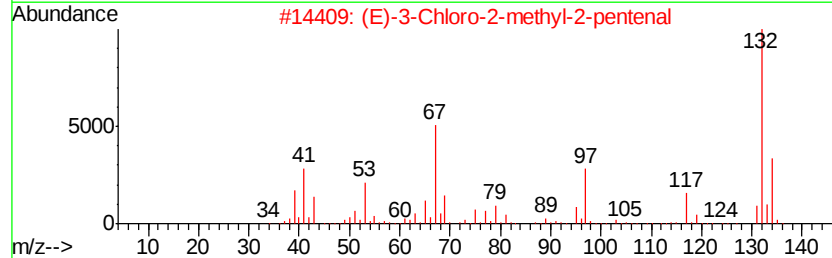
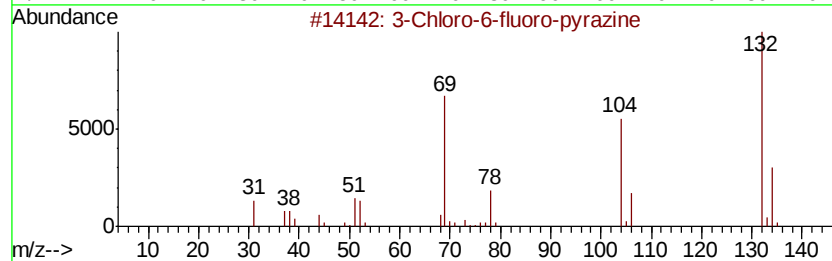
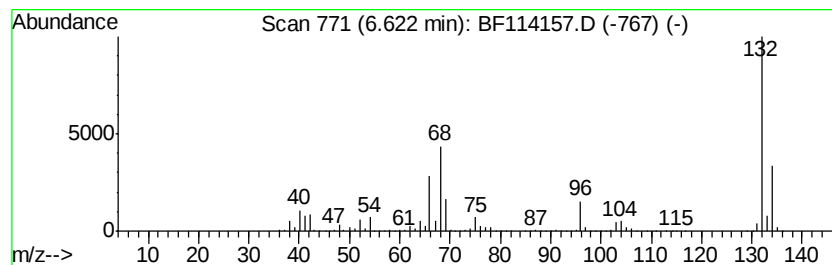
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	68.37 ng	5456350	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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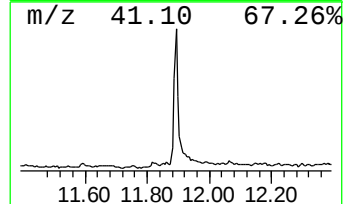
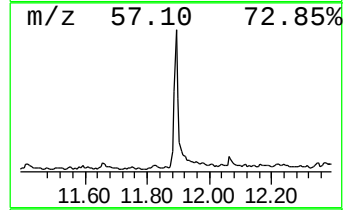
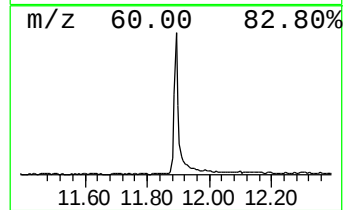
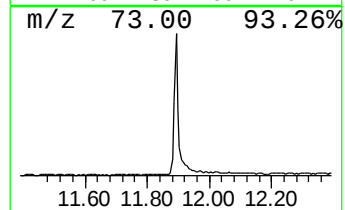
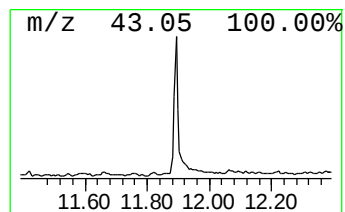
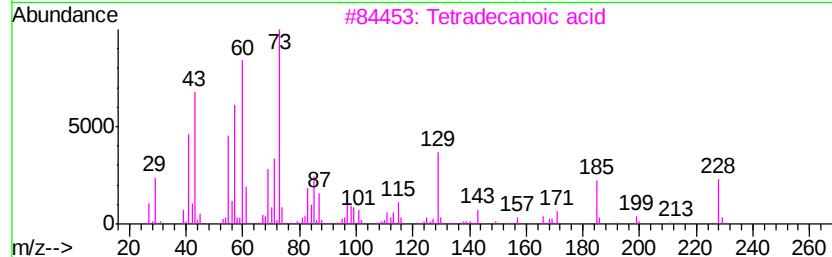
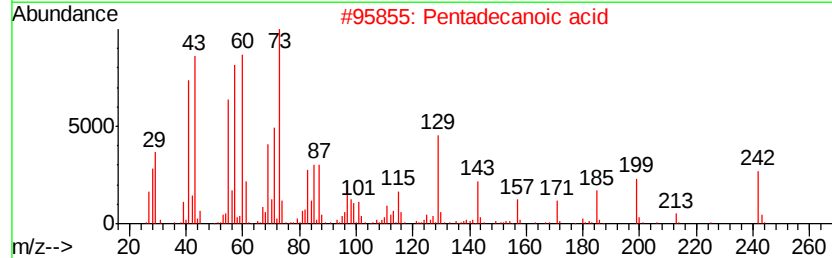
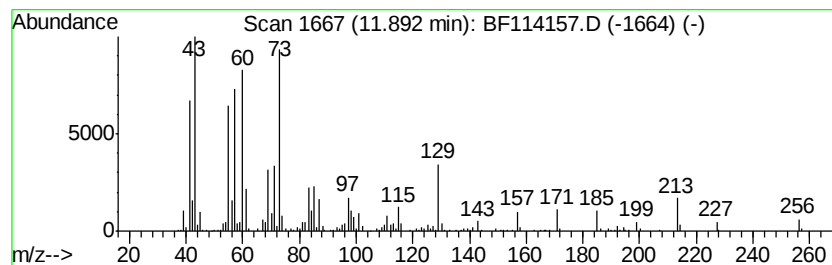
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	6.01 ng	713759	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99	
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	78	
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74	
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74	
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59	



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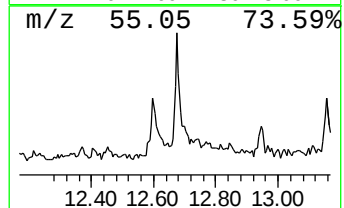
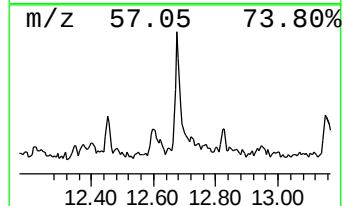
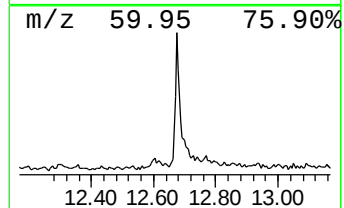
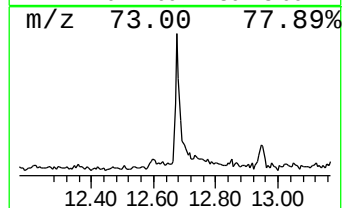
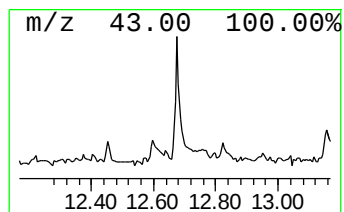
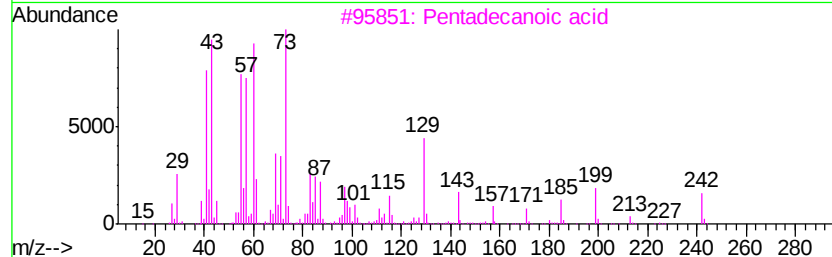
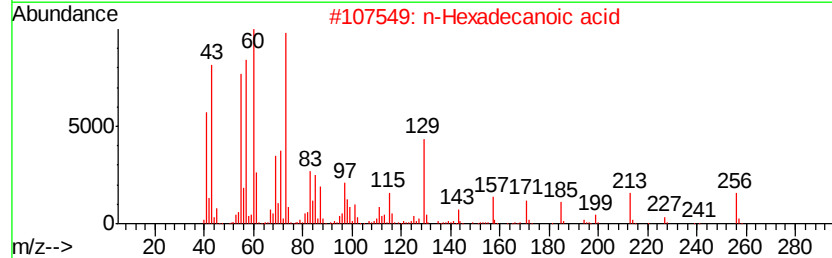
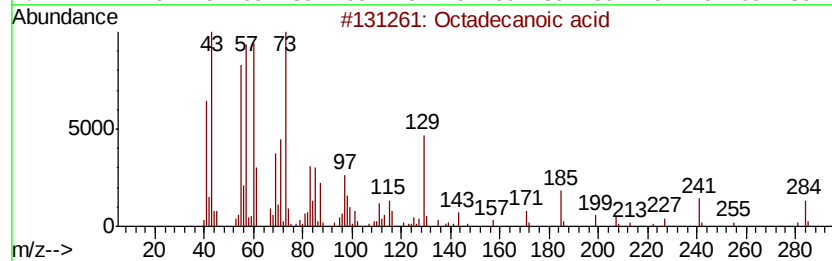
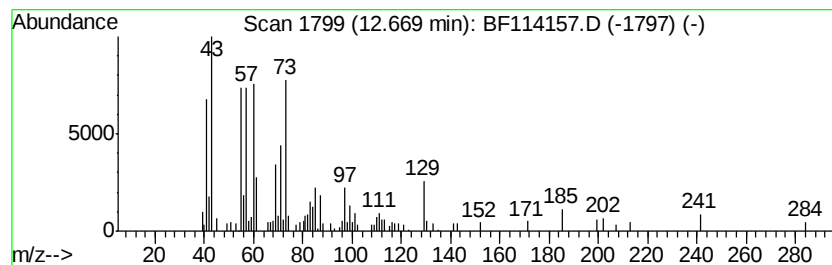
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.67	2.02 ng	239824	Phenanthrene-d10	11.37	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	52
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	52



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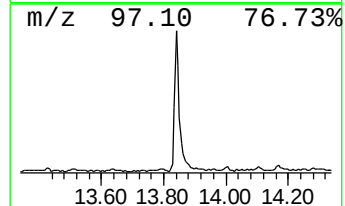
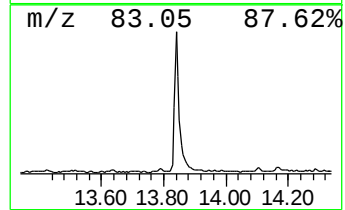
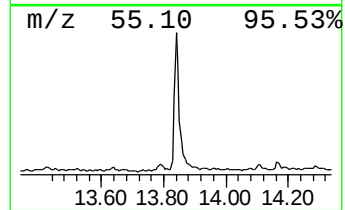
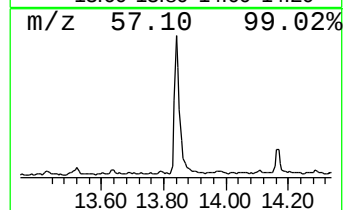
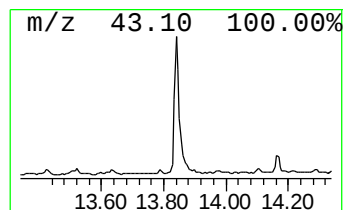
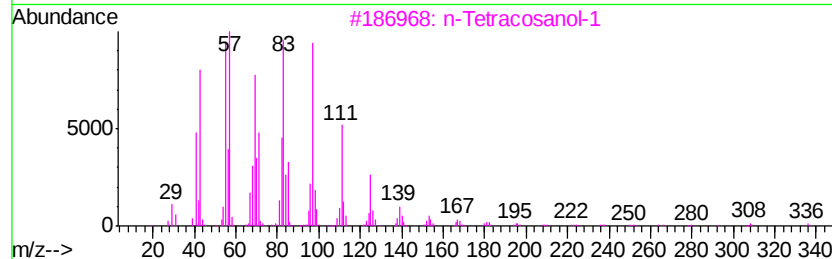
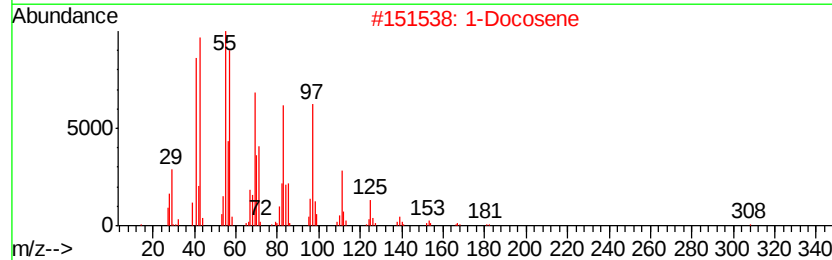
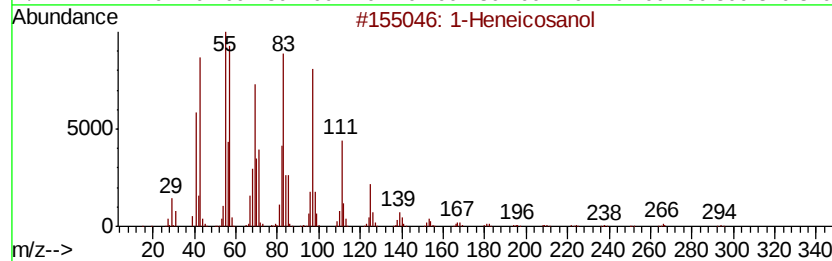
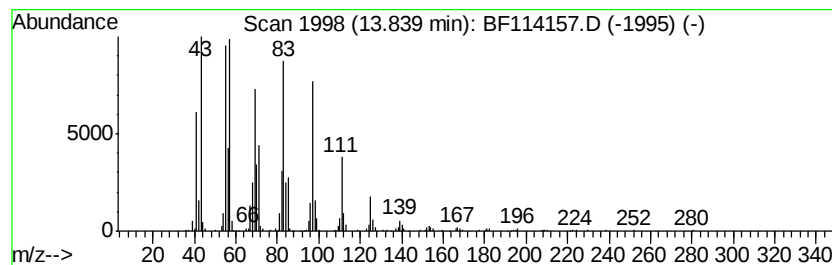
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	14.75 ng	1184190	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		1-Docosene	308	C22H44	001599-67-3	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	91
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	91



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ALS Vial : 10 Sample Multiplier: 1

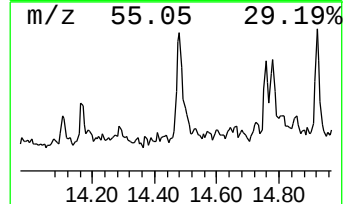
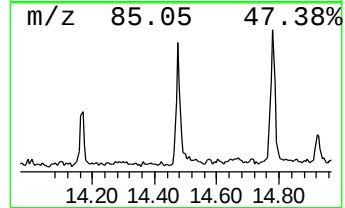
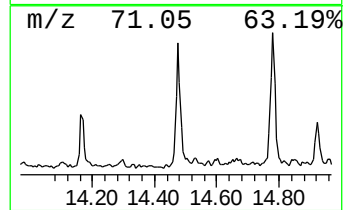
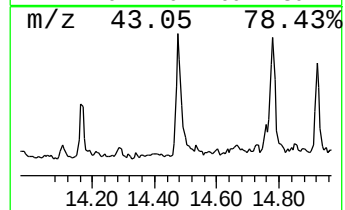
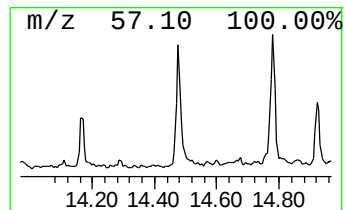
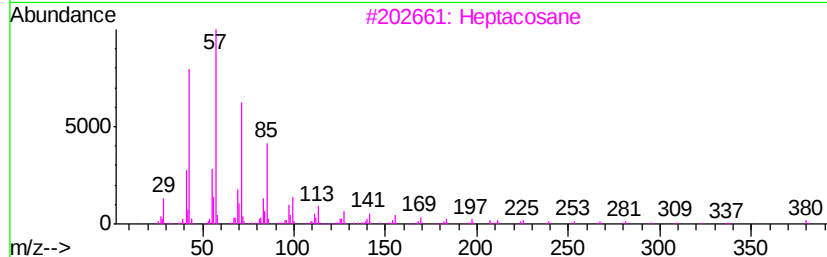
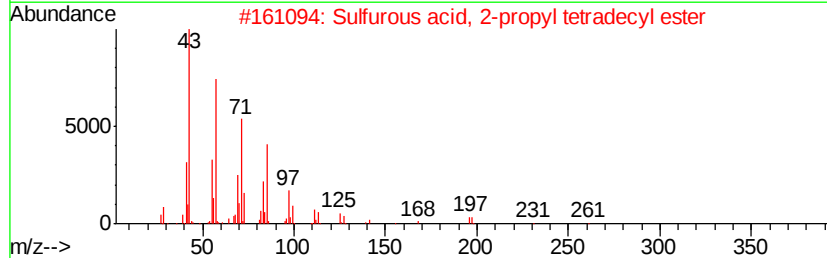
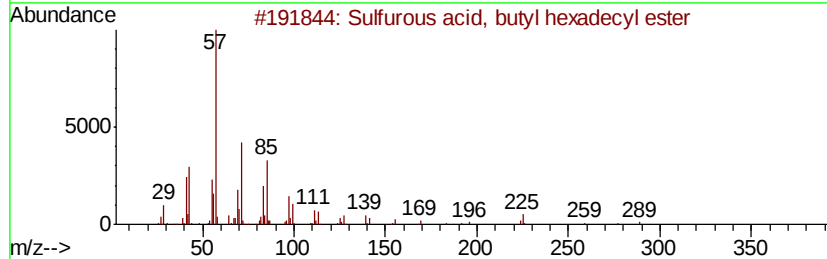
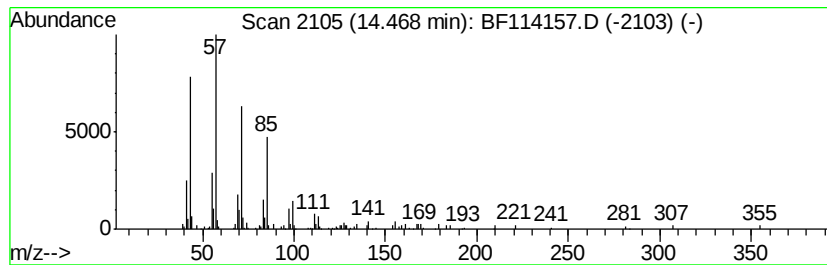
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl hexad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.47	3.27 ng	262259	Chrysene-d12	14.00		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	91
2		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	91
3		Heptacosane	380	C27H56	000593-49-7	87
4		Octadecane	254	C18H38	000593-45-3	86
5		2-methyloctacosane	408	C29H60	1000376-72-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114157.D
Acq On : 11 May 2019 15:21
Operator : JU/SJ
Sample : K2763-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

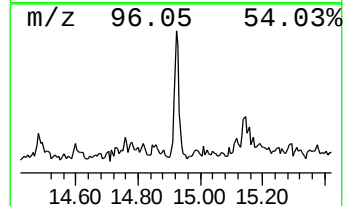
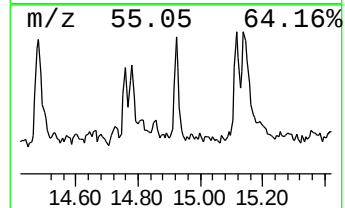
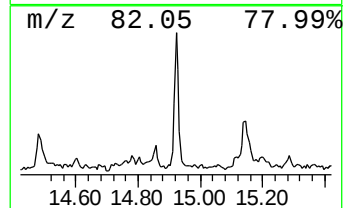
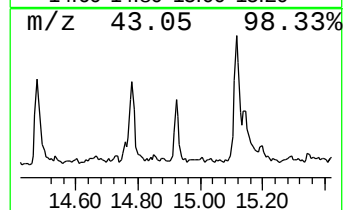
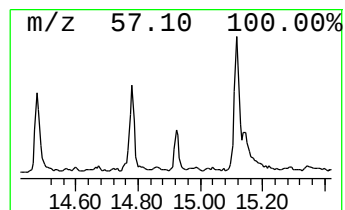
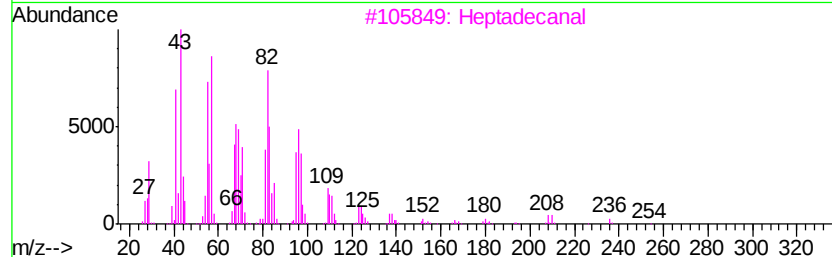
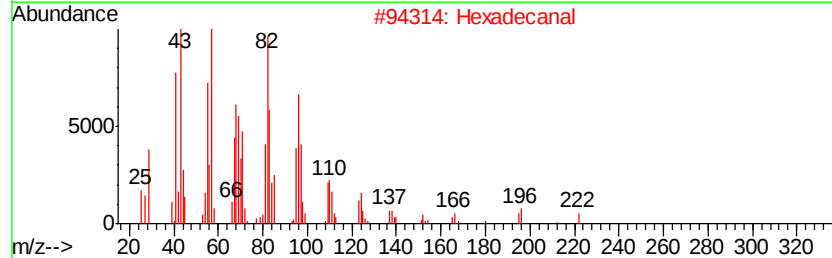
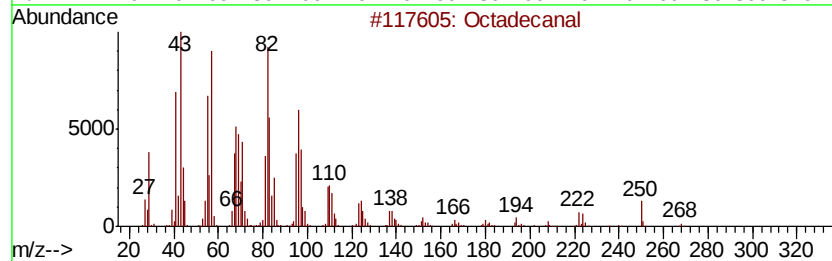
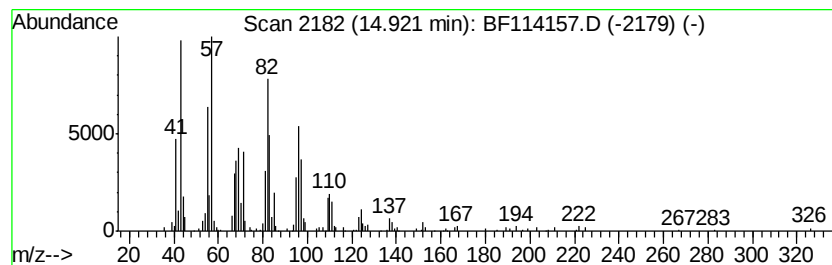
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.92	2.40 ng	204444	Perylene-d12		15.47
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Hexadecanal	240	C16H32O	000629-80-1	91
3	Heptadecanal	254	C17H34O	1000376-70-0	87
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	83
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
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Sample : K2763-04
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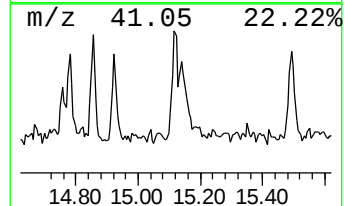
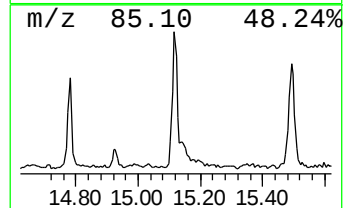
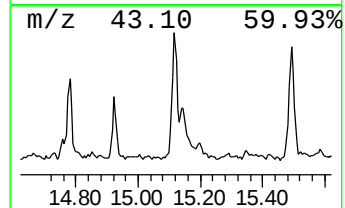
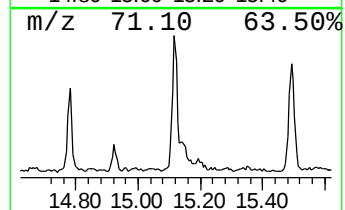
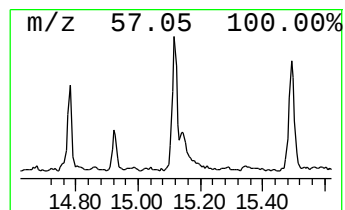
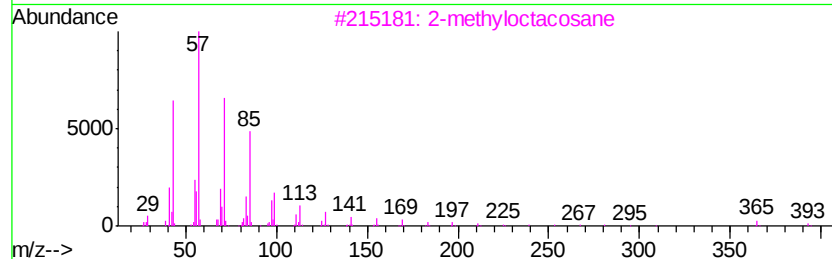
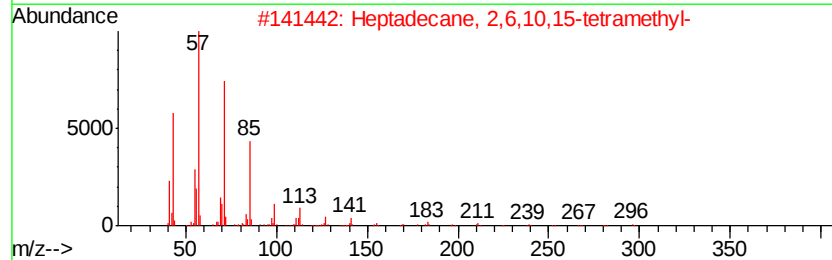
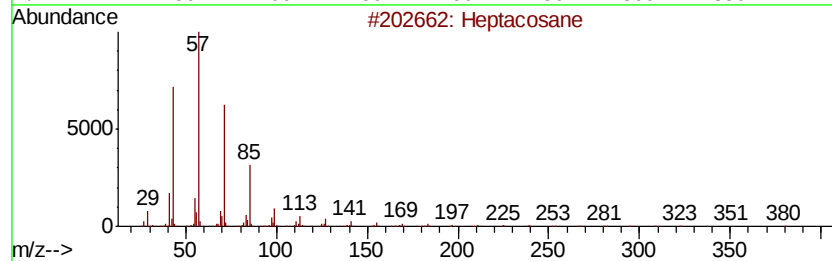
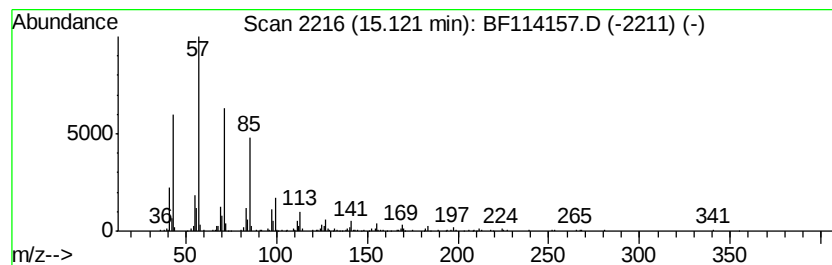
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	4.29 ng	365245	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6	91
3	2-methyloctacosane	408 C29H60	1000376-72-8	91
4	Hexacosane	366 C26H54	000630-01-3	91
5	2-Bromo dodecane	248 C12H25Br	013187-99-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114157.D
Acq On : 11 May 2019 15:21
Operator : JU/SJ
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Instrument :
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ClientSampleId :
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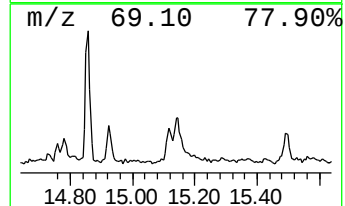
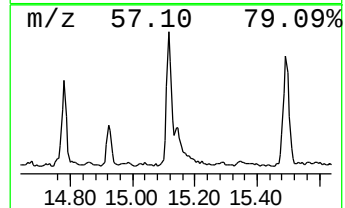
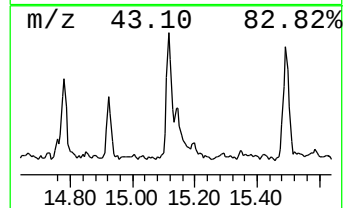
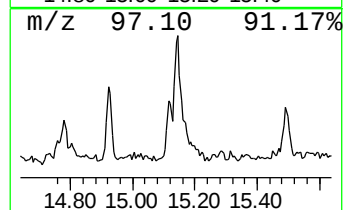
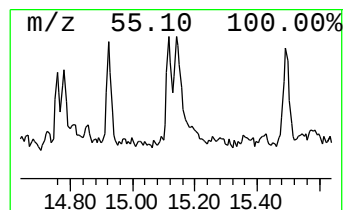
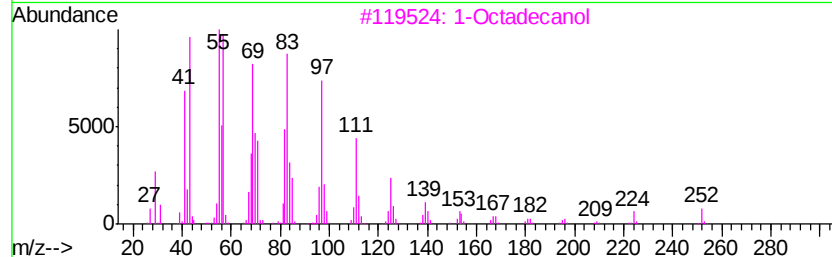
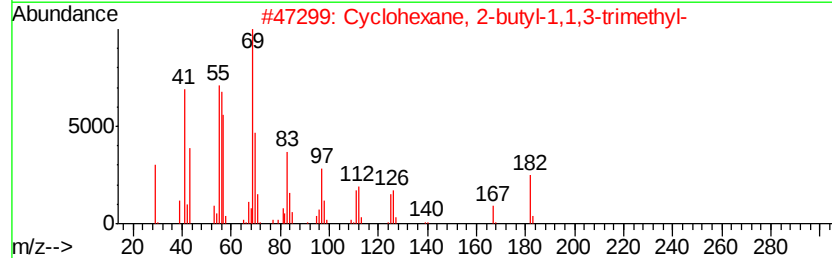
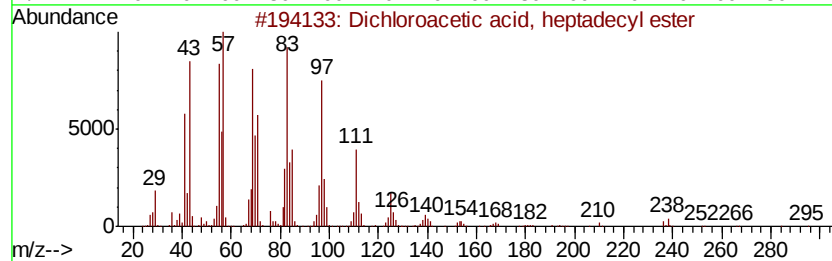
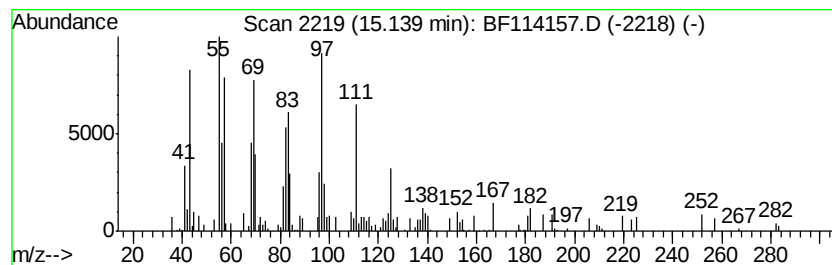
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dichloroacetic acid, heptad... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	2.37 ng	201361	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	59
2		Cyclohexane, 2-butyl-1,1,3-trime...	182	C13H26	054676-39-0	58
3		1-Octadecanol	270	C18H38O	000112-92-5	53
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	52
5		trans-1,3-Diethylcyclopentane	126	C9H18	1000113-87-1	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
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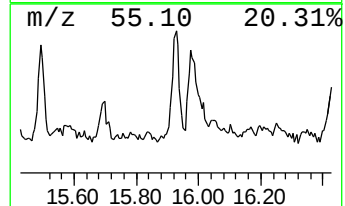
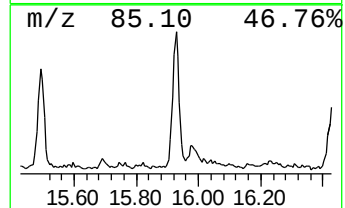
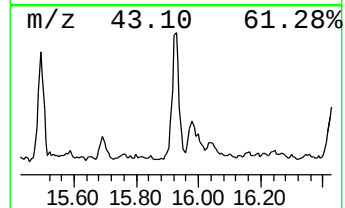
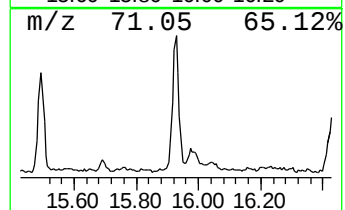
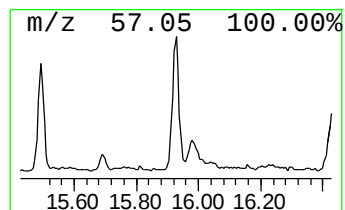
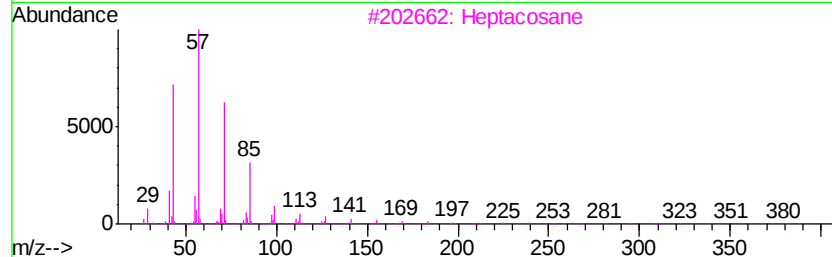
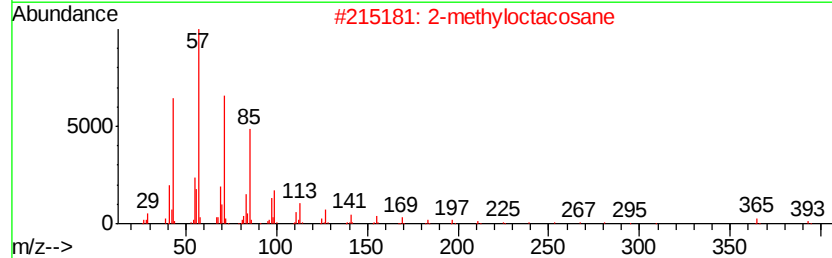
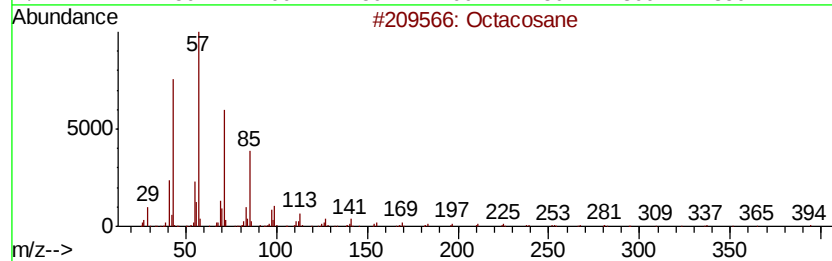
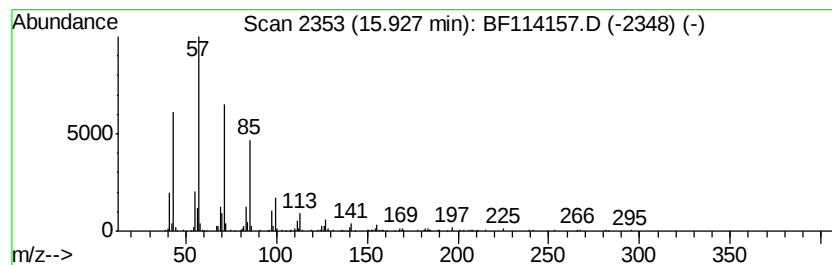
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	5.61 ng	477159	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		Heneicosane	296	C21H44	000629-94-7	90



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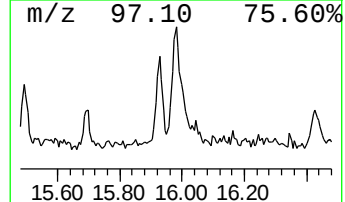
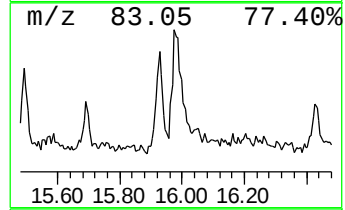
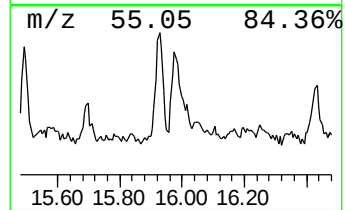
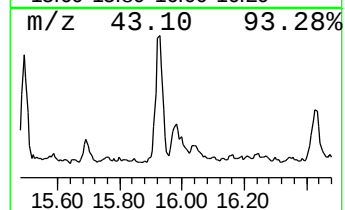
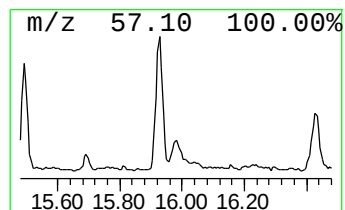
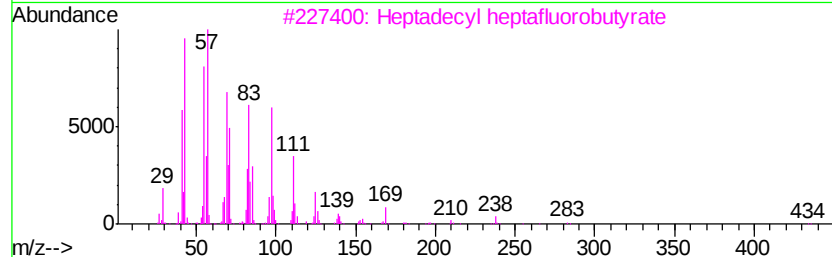
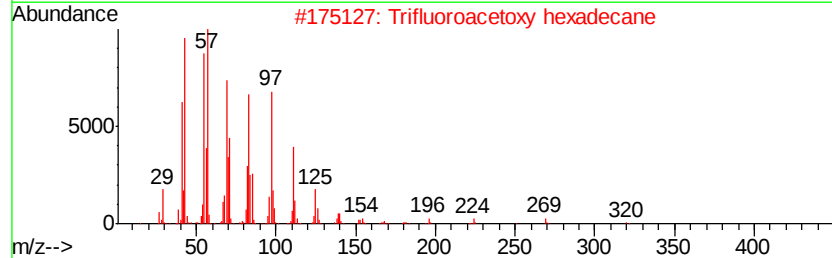
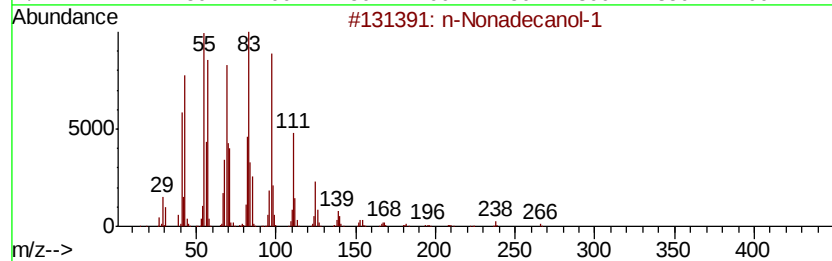
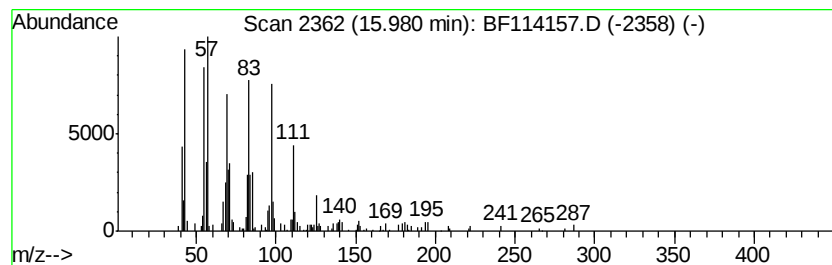
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Nonadecanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.82 ng	240144	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Nonadecanol-1	284 C19H40O	001454-84-8	94
2	Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3	94
3	Heptadecyl heptafluorobutyrat	452 C21H35F7O2	959085-66-6	91
4	Heptadecyl trifluoroacetate	352 C19H35F3O2	1000351-87-0	91
5	1-Octadecanol	270 C18H38O	000112-92-5	91



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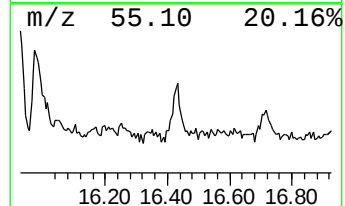
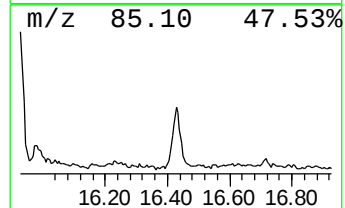
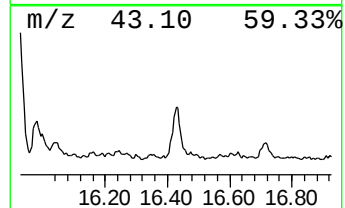
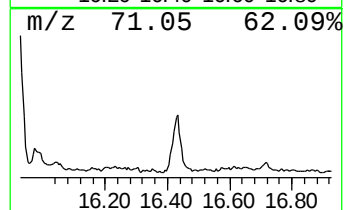
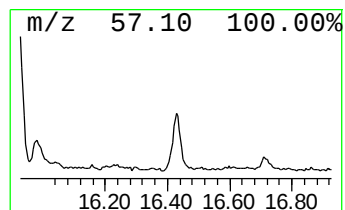
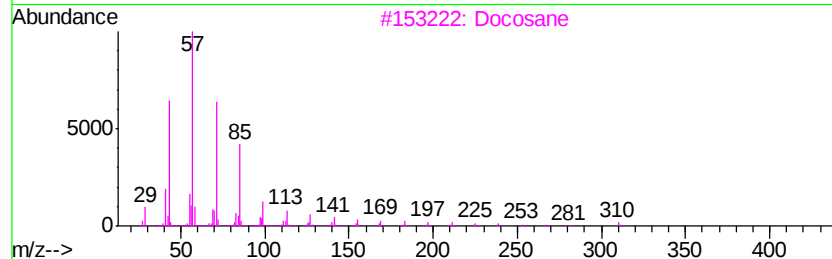
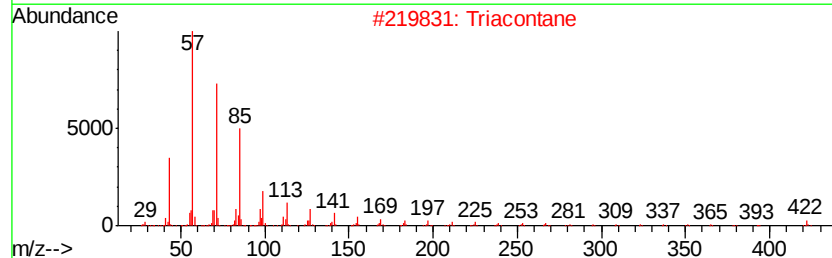
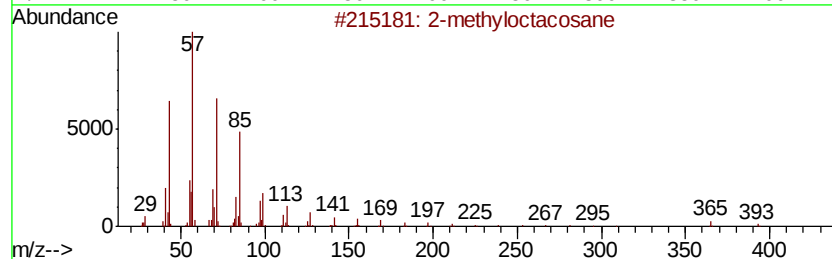
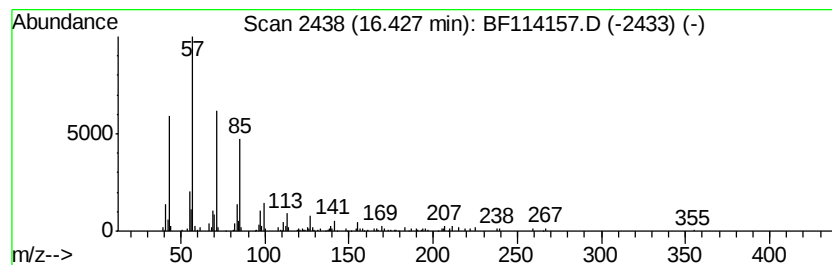
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	2.79 ng	237634	Perylene-d12	15.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	87
2			Triacontane	422	C30H62	000638-68-6	86
3			Docosane	310	C22H46	000629-97-0	86
4			Tetracosane	338	C24H50	000646-31-1	86
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051119\
 Data File : BF114157.D
 Acq On : 11 May 2019 15:21
 Operator : JU/SJ
 Sample : K2763-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P021-SS005-0206-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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
2-Pentanone, 4-hy...	5.06	3.6 ng		289039	1	6.85	1596240	20.0
unknown6.62	6.62	68.4 ng		5456350	1	6.85	1596240	20.0
n-Hexadecanoic acid	11.89	6.0 ng		713759	4	11.37	2375620	20.0
Octadecanoic acid	12.67	2.0 ng		239824	4	11.37	2375620	20.0
1-Heneicosanol	13.84	14.8 ng		1184190	5	14.00	1605570	20.0
Sulfurous acid, b...	14.47	3.3 ng		262259	5	14.00	1605570	20.0
Octadecanal	14.92	2.4 ng		204444	6	15.47	1701790	20.0
Heptacosane	15.12	4.3 ng		365245	6	15.47	1701790	20.0
Dichloroacetic ac...	15.14	2.4 ng		201361	6	15.47	1701790	20.0
Octacosane	15.93	5.6 ng		477159	6	15.47	1701790	20.0
n-Nonadecanol-1	15.98	2.8 ng		240144	6	15.47	1701790	20.0
2-methyloctacosane	16.43	2.8 ng		237634	6	15.47	1701790	20.0