

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
 Data File : BF114155.D
 Acq On : 11 May 2019 14:28
 Operator : JU/SJ
 Sample : K2763-08
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P021-SS006-0002-01

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	2.146	4	10	27	rVB	1759557	2636899	31.85%	3.241%
2	5.481	572	577	581	rBV	6925138	7385134	89.21%	9.076%
3	6.492	743	749	752	rBV	7517108	7925004	95.73%	9.740%
4	6.628	767	772	775	rBV	8001236	7745576	93.56%	9.519%
5	6.851	806	810	813	rBV	2250484	1760393	21.26%	2.164%
6	7.010	832	837	840	rBV	6786943	5946214	71.83%	7.308%
7	7.410	900	905	908	rBV	5509805	5453043	65.87%	6.702%
8	7.451	908	912	915	rVB	173273	161458	1.95%	0.198%
9	8.128	1023	1027	1031	rBV	2893720	2481032	29.97%	3.049%
10	8.816	1141	1144	1151	rBV	123065	131594	1.59%	0.162%
11	9.204	1205	1210	1213	rBV	8871310	8278409	100.00%	10.174%
12	9.592	1273	1276	1280	rBV	1005276	765333	9.24%	0.941%
13	9.798	1305	1311	1316	rVB2	145333	143945	1.74%	0.177%
14	9.880	1321	1325	1329	rBV	3090223	2759161	33.33%	3.391%
15	10.669	1455	1459	1463	rBV	5193853	5434958	65.65%	6.680%
16	11.369	1573	1578	1580	rBV	2973761	2875878	34.74%	3.534%
17	11.386	1580	1581	1584	rVB	137419	103155	1.25%	0.127%
18	11.892	1664	1667	1671	rBV	901219	801442	9.68%	0.985%
19	12.574	1780	1783	1786	rBV	333721	332879	4.02%	0.409%
20	12.598	1786	1787	1793	rVV	139686	118459	1.43%	0.146%
21	12.674	1797	1800	1812	rBV	477297	595447	7.19%	0.732%
22	12.804	1817	1822	1828	rVB	280318	297792	3.60%	0.366%
23	12.951	1842	1847	1850	rBV	7143424	6753161	81.58%	8.300%
24	13.474	1933	1936	1939	rBV	130235	115151	1.39%	0.142%
25	13.792	1986	1990	1995	rBV5	67978	105757	1.28%	0.130%
26	13.845	1995	1999	2006	rVB2	379863	530606	6.41%	0.652%
27	14.004	2020	2026	2029	rBV	2062798	2048386	24.74%	2.517%
28	14.162	2050	2053	2056	rBV	143747	138155	1.67%	0.170%
29	14.474	2102	2106	2112	rBV2	341466	384900	4.65%	0.473%
30	14.709	2143	2146	2151	rBV	84918	102483	1.24%	0.126%
31	14.757	2151	2154	2155	rVV	108821	102286	1.24%	0.126%
32	14.780	2155	2158	2166	rVB	384660	443612	5.36%	0.545%
33	14.921	2179	2182	2186	rVB	244226	222180	2.68%	0.273%
34	15.039	2199	2202	2206	rBV	92105	138356	1.67%	0.170%

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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

35	15.115	2210	2215	2218	rBV	588342	733643	8.86%	0.902%
36	15.139	2218	2219	2226	rVB3	180087	199593	2.41%	0.245%
37	15.339	2250	2253	2261	rBV2	76591	134847	1.63%	0.166%
38	15.404	2261	2264	2270	rVB	86080	104753	1.27%	0.129%
39	15.468	2270	2275	2278	rBV	1633077	2181882	26.36%	2.682%
40	15.692	2310	2313	2318	rVB3	98777	122703	1.48%	0.151%
41	15.927	2347	2353	2358	rBV	612423	924749	11.17%	1.137%
42	16.427	2433	2438	2444	rVB	274150	452277	5.46%	0.556%
43	16.715	2482	2487	2493	rBV3	116279	214387	2.59%	0.263%
44	16.921	2519	2522	2531	rBV3	43721	108309	1.31%	0.133%
45	17.015	2534	2538	2545	rVB2	123156	252378	3.05%	0.310%
46	17.221	2568	2573	2577	rBV3	130819	261691	3.16%	0.322%
47	17.274	2577	2582	2589	rVB4	220733	458065	5.53%	0.563%

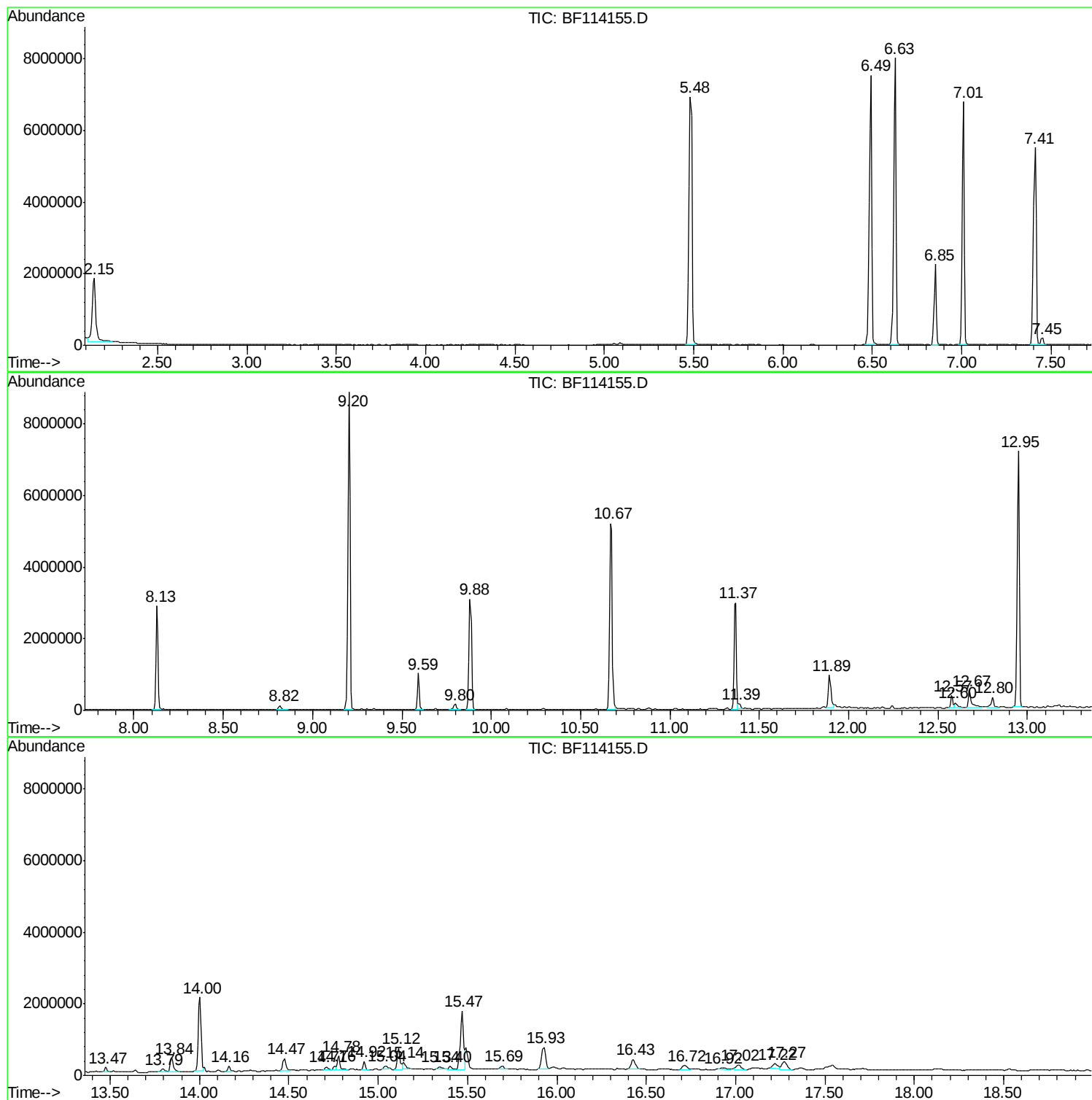
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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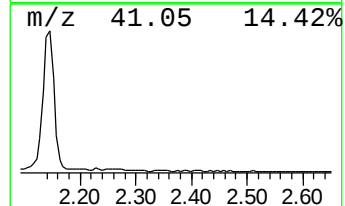
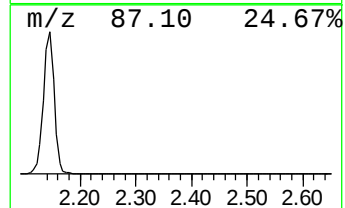
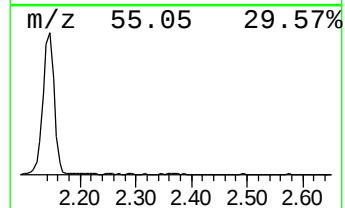
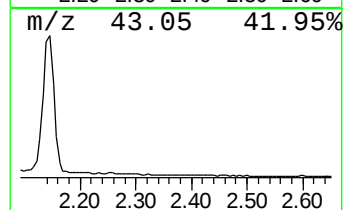
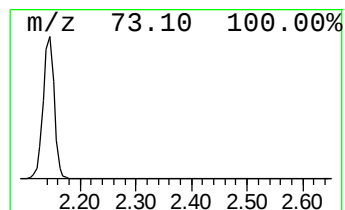
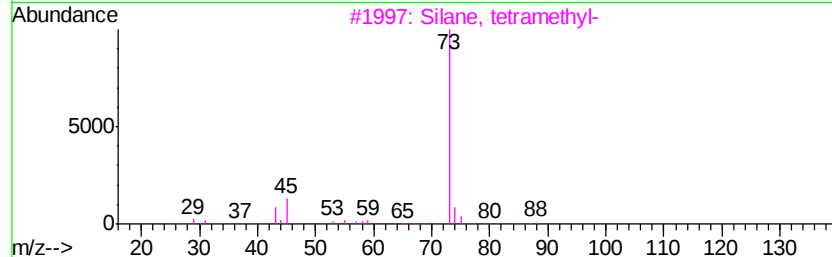
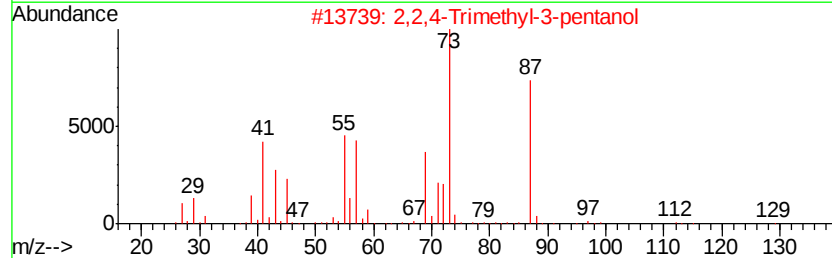
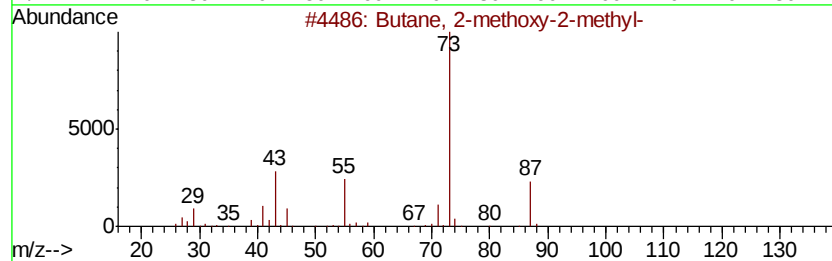
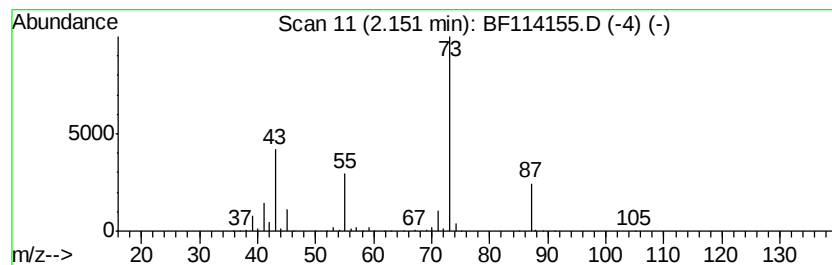
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	29.96 ng	2636900	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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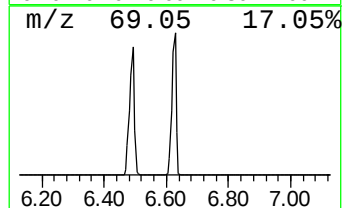
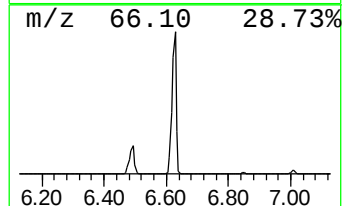
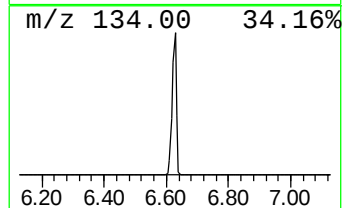
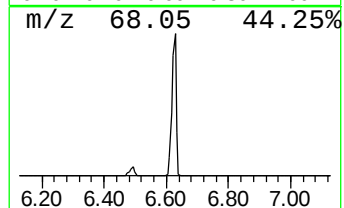
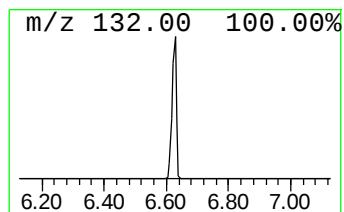
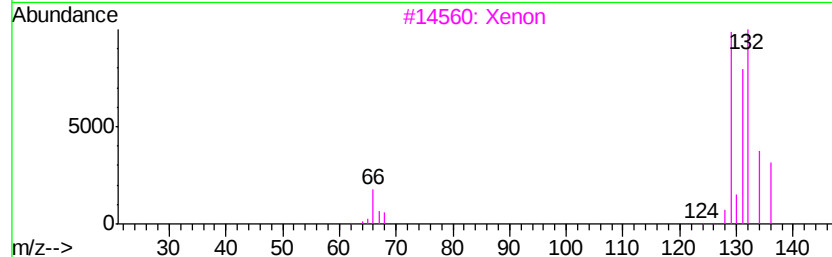
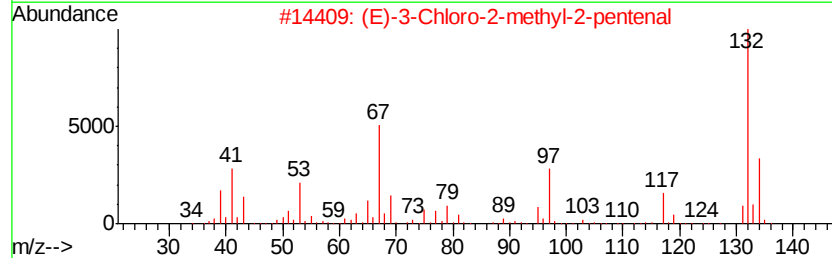
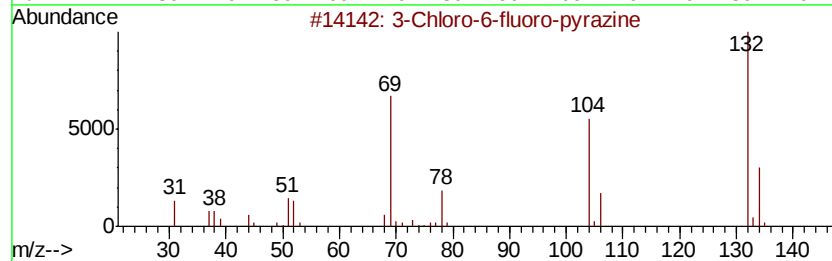
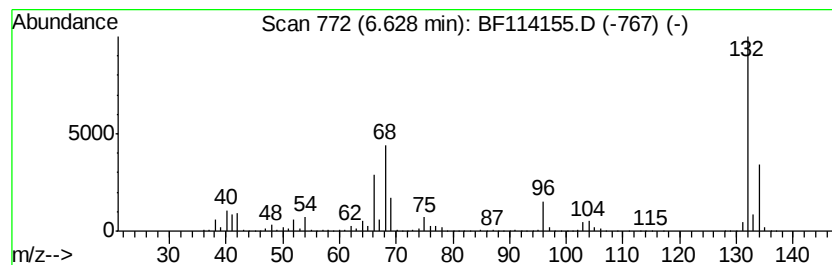
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	88.00 ng	7745580	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Xenon	132	Xe	007440-63-3	9	
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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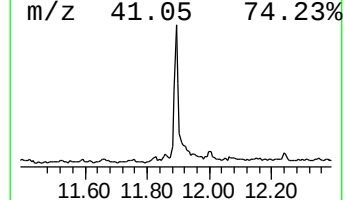
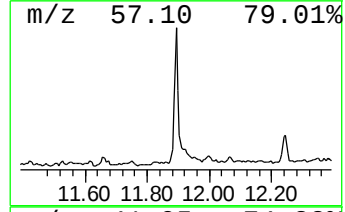
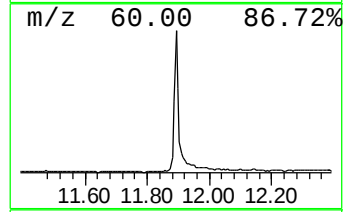
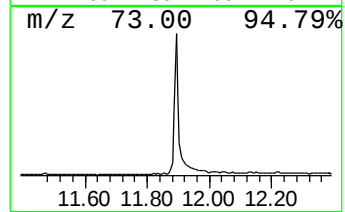
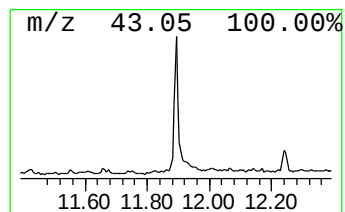
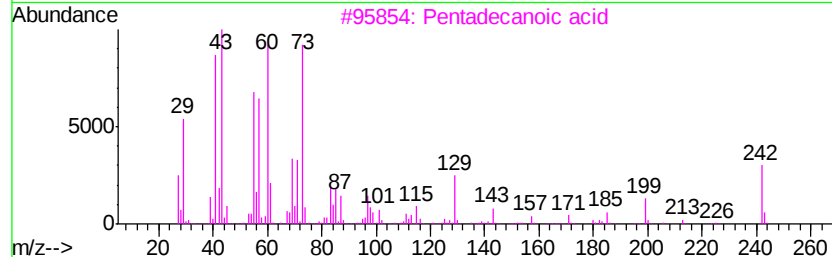
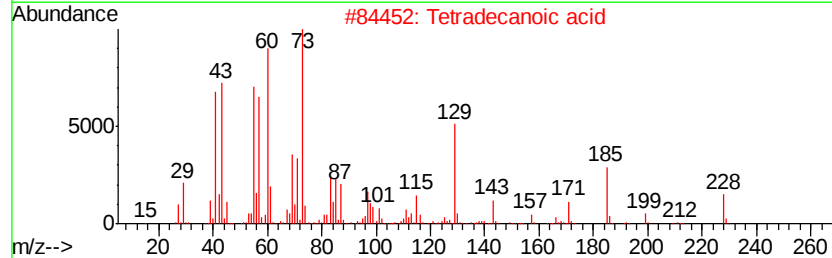
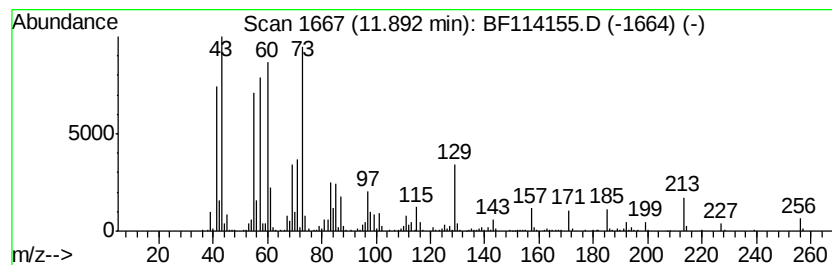
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	5.57 ng	801442	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	59



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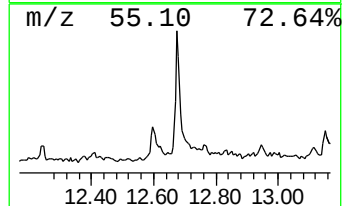
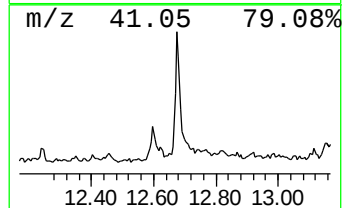
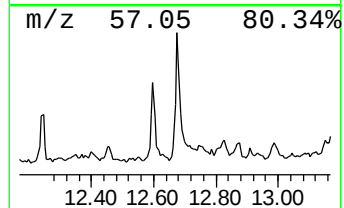
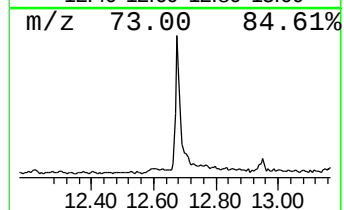
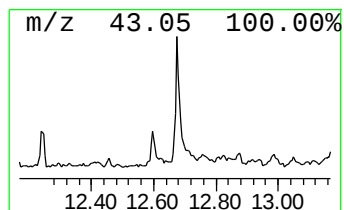
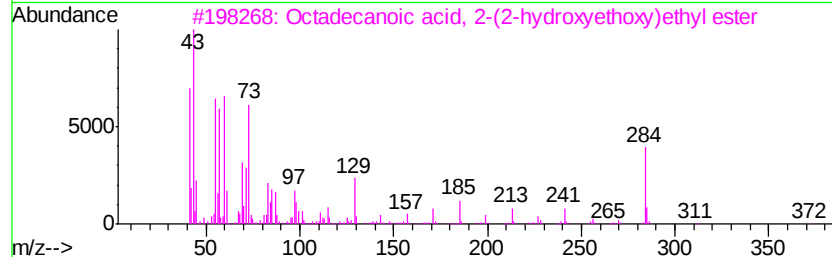
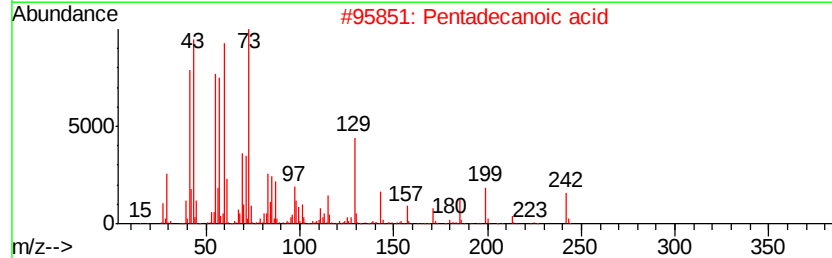
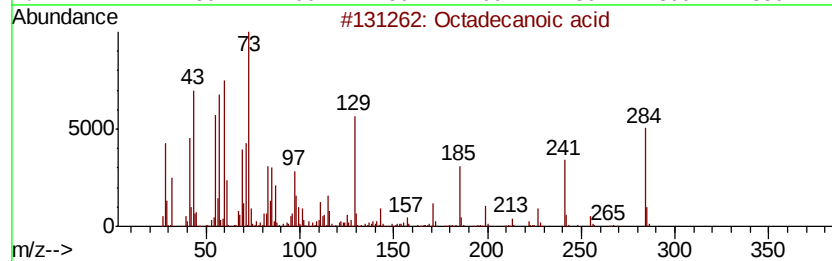
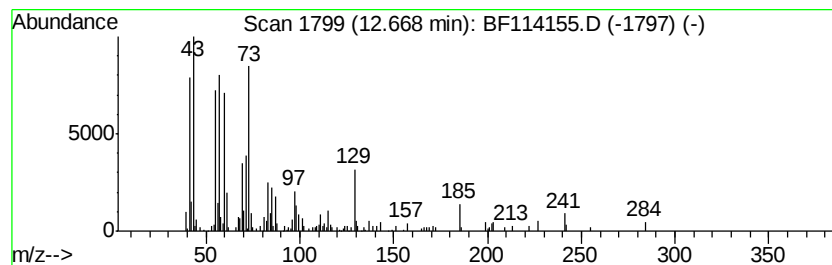
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	4.14 ng	595447	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5		Tridecanoic acid	214	C13H26O2	000638-53-9	58



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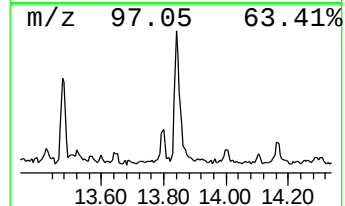
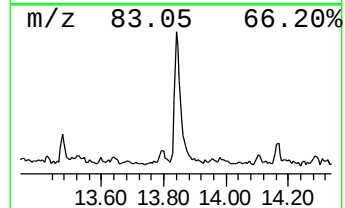
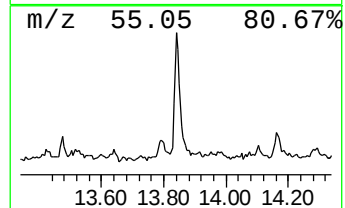
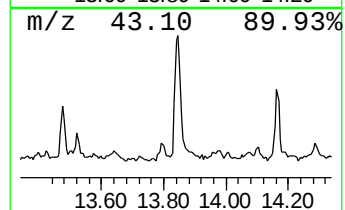
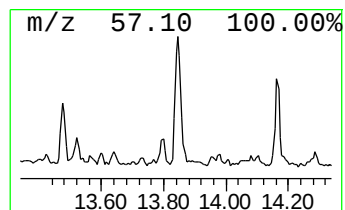
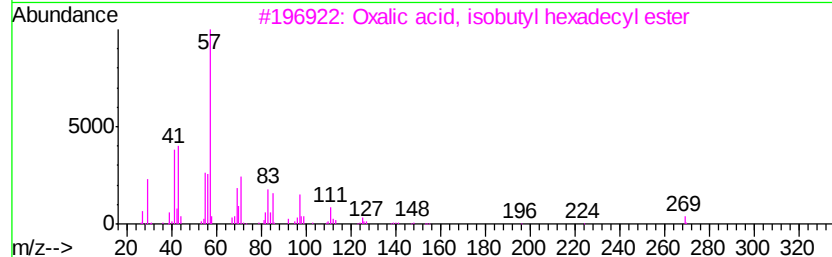
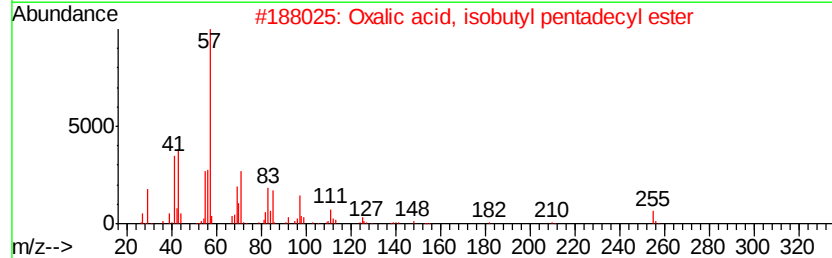
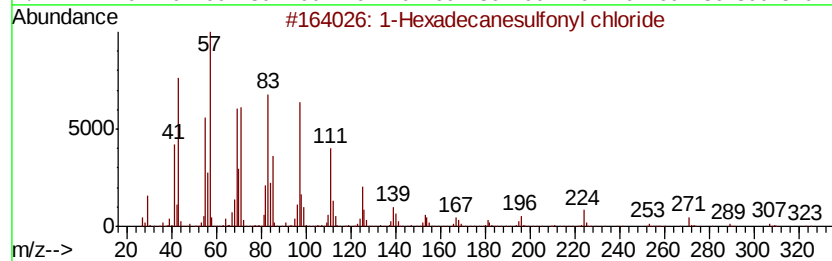
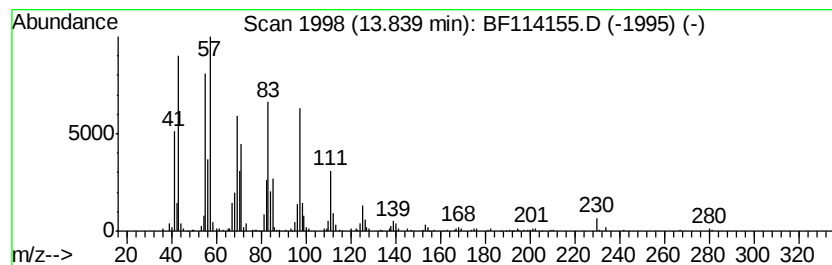
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 1-Hexadecanesulfonyl chloride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	5.18 ng	530606	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
3		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
4		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87
5		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114155.D
Acq On : 11 May 2019 14:28
Operator : JU/SJ
Sample : K2763-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

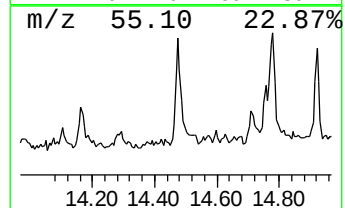
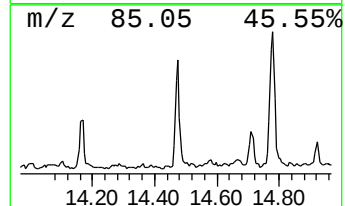
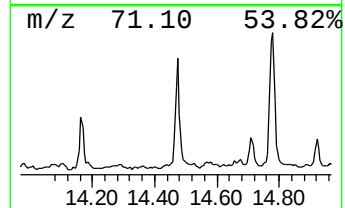
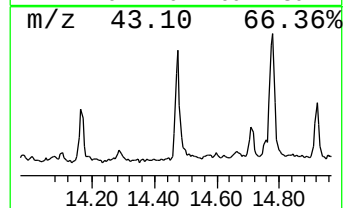
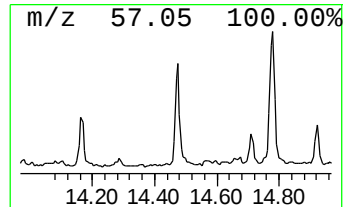
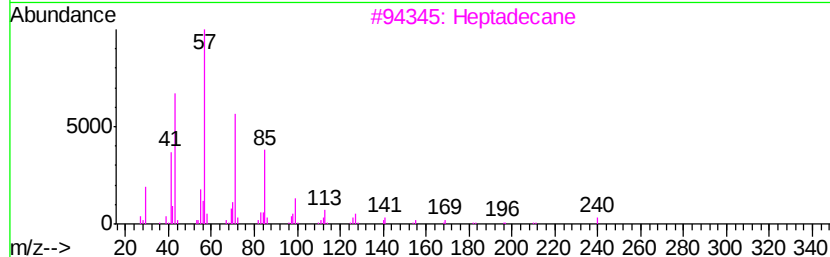
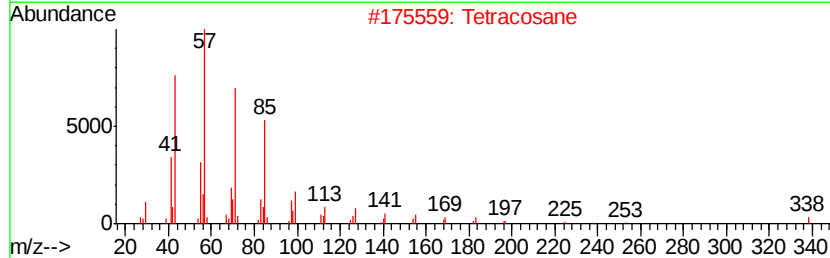
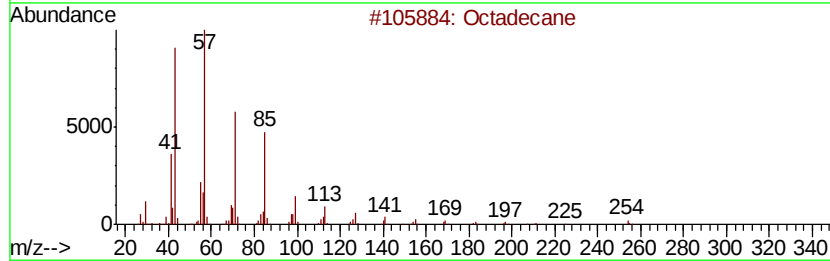
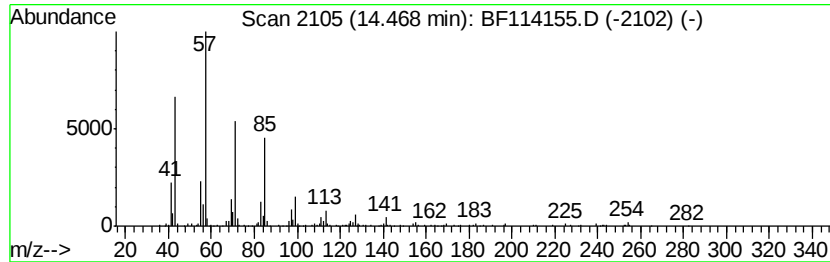
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.47	3.76 ng	384900	Chrysene-d12		14.00		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	98
2			Tetracosane	338	C24H50	000646-31-1	91
3			Heptadecane	240	C17H36	000629-78-7	91
4			Octacosane	394	C28H58	000630-02-4	90
5			2-methyloctacosane	408	C29H60	1000376-72-8	90



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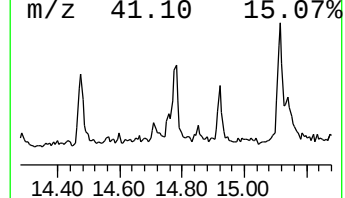
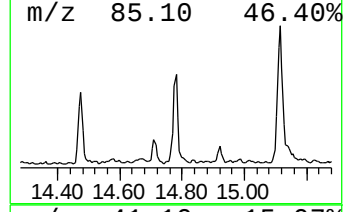
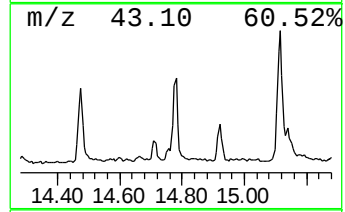
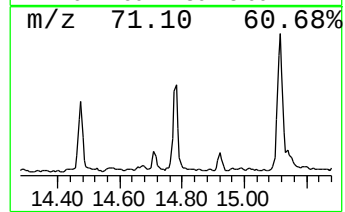
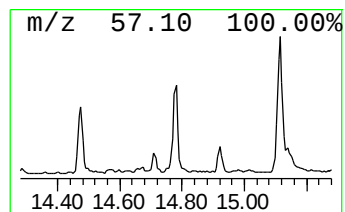
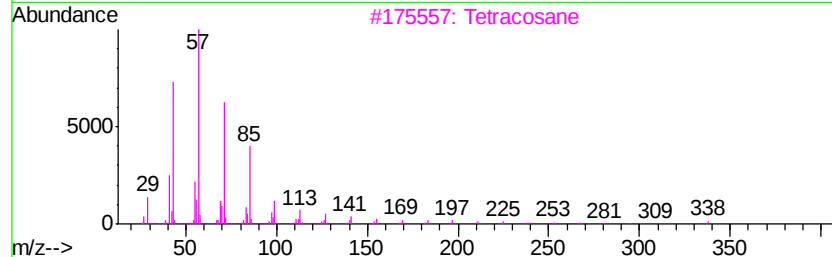
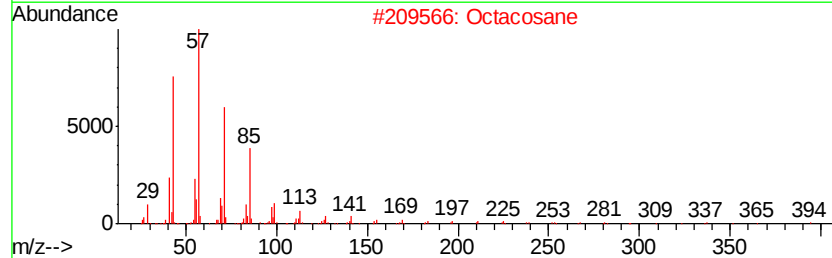
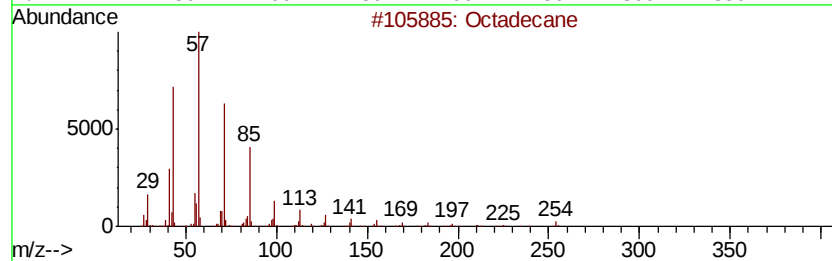
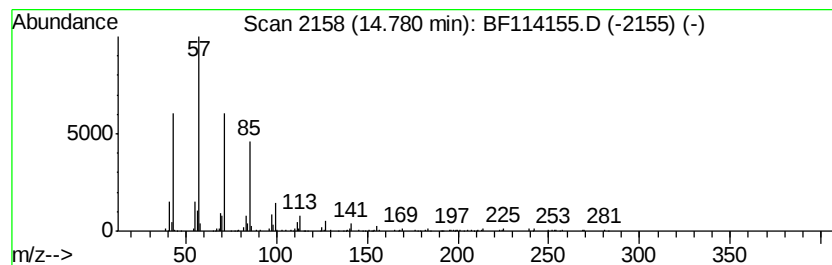
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	4.07 ng	443612	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	90
2	Octacosane	394 C28H58	000630-02-4	90
3	Tetracosane	338 C24H50	000646-31-1	90
4	Heneicosane	296 C21H44	000629-94-7	86
5	Octadecane, 1-iodo-	380 C18H37I	000629-93-6	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
 Data File : BF114155.D
 Acq On : 11 May 2019 14:28
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Instrument :
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 ClientSampleId :
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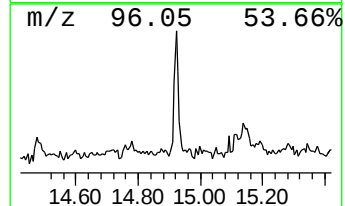
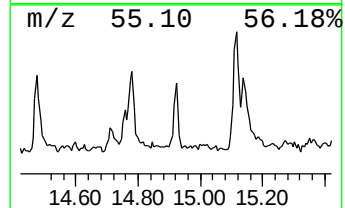
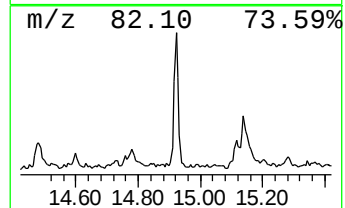
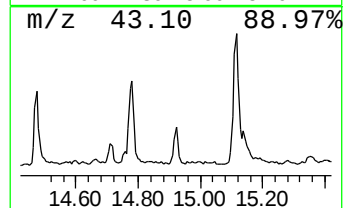
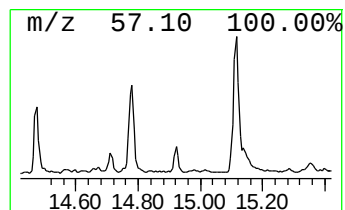
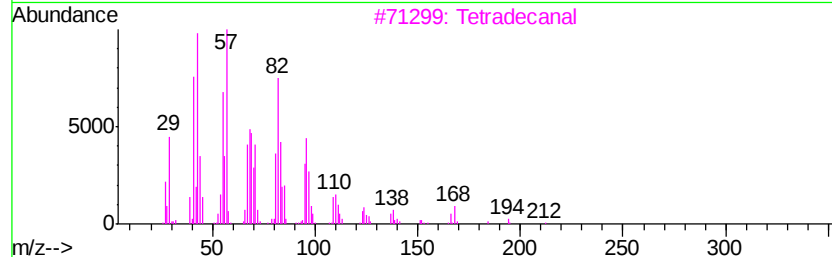
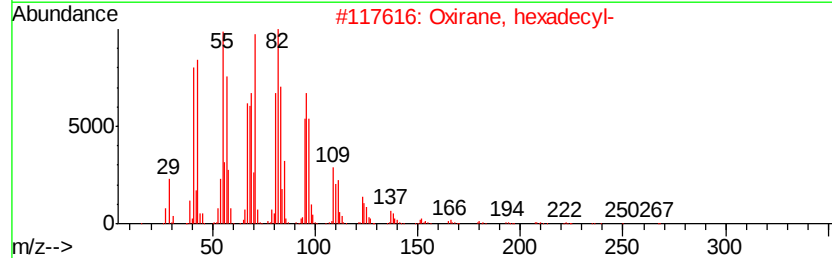
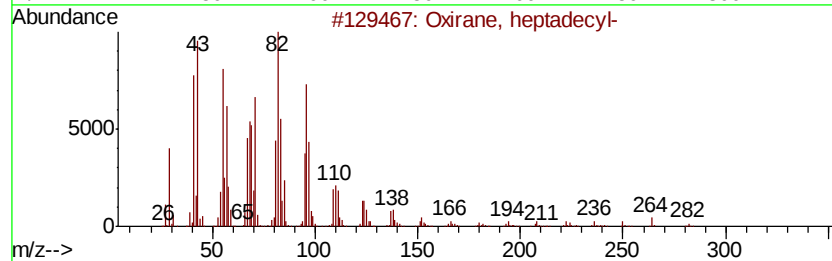
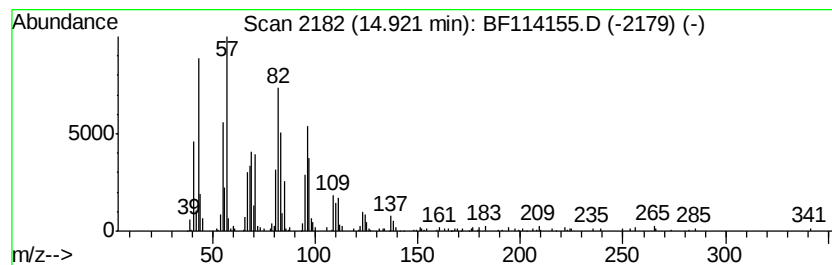
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 10 Oxirane, heptadecyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.04 ng	222180	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3		Tetradecanal	212	C14H28O	000124-25-4	90
4		Octadecanal	268	C18H36O	000638-66-4	86
5		15-Octadecenal	266	C18H34O	056554-93-9	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
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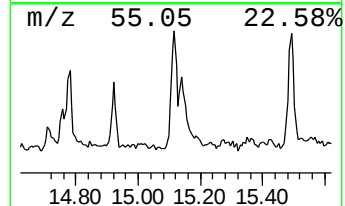
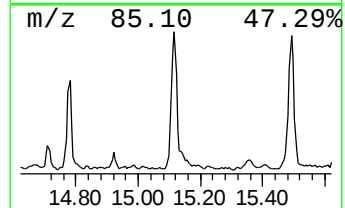
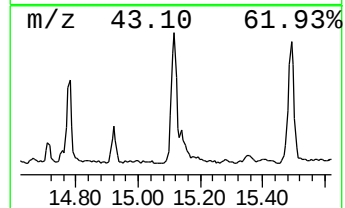
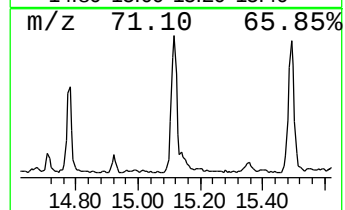
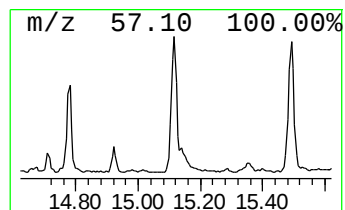
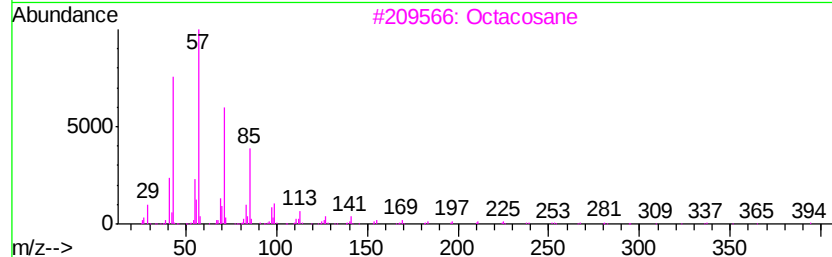
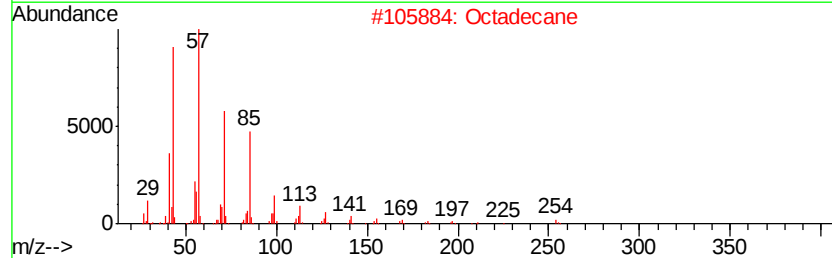
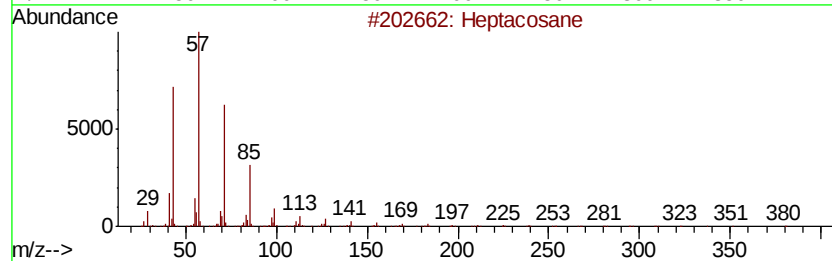
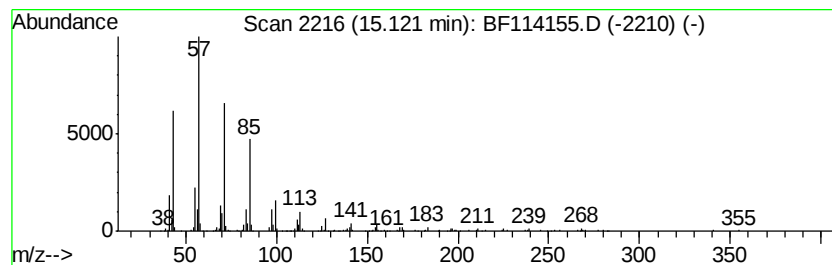
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	6.72 ng	733643	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Octadecane	254	C18H38	000593-45-3	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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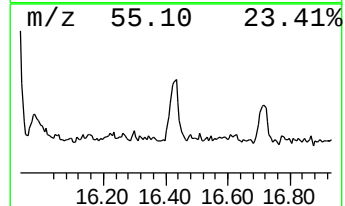
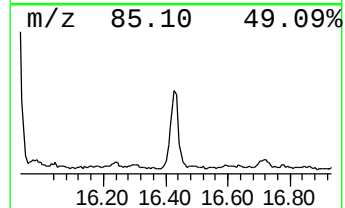
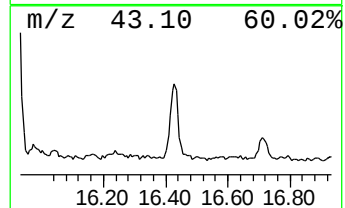
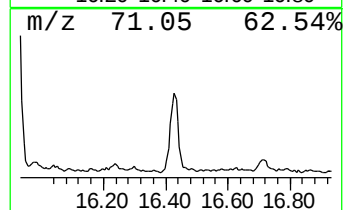
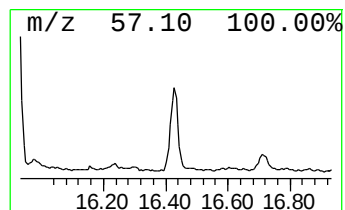
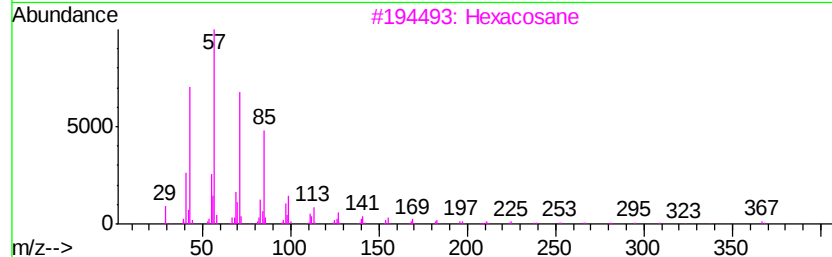
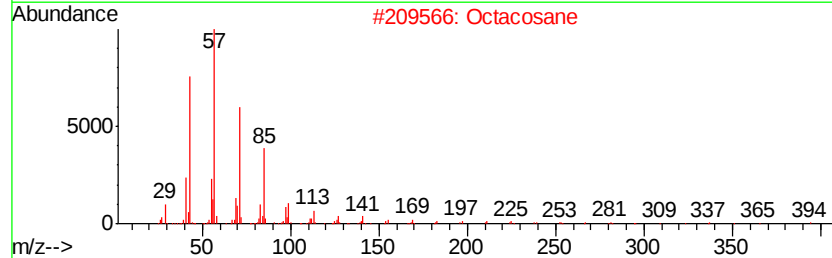
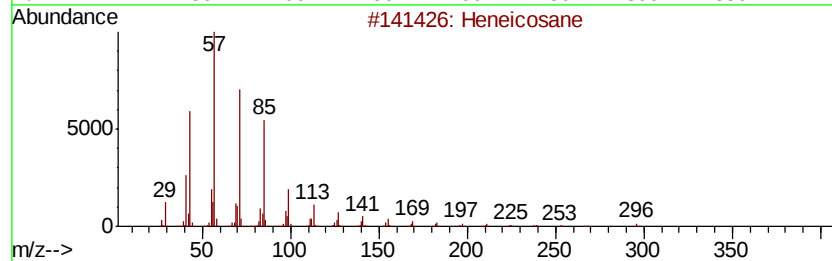
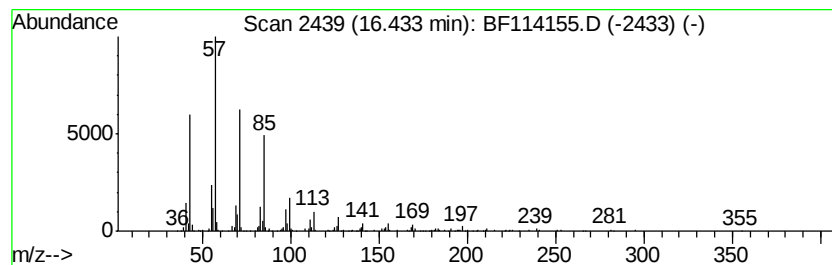
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	4.15 ng	452277	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Octacosane	394	C28H58	000630-02-4	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114155.D
Acq On : 11 May 2019 14:28
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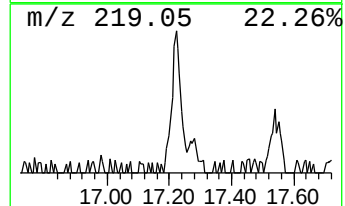
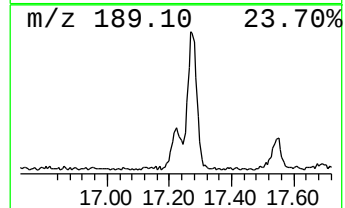
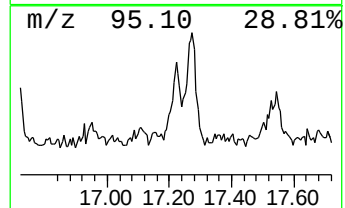
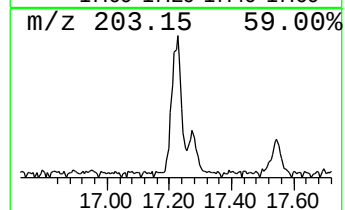
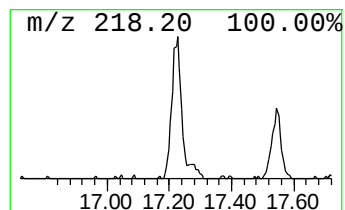
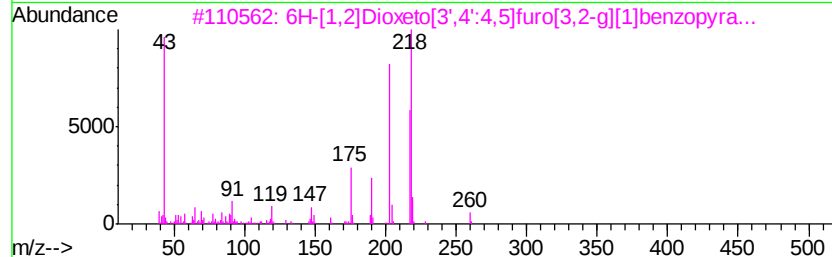
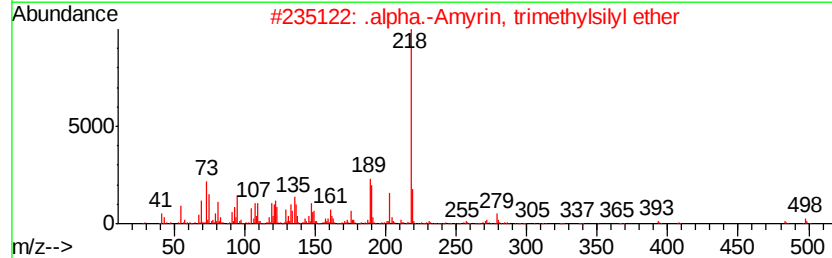
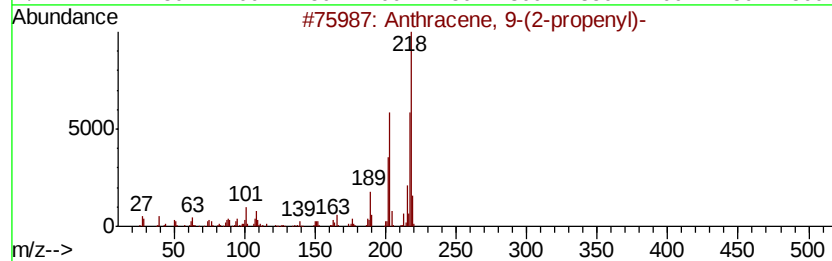
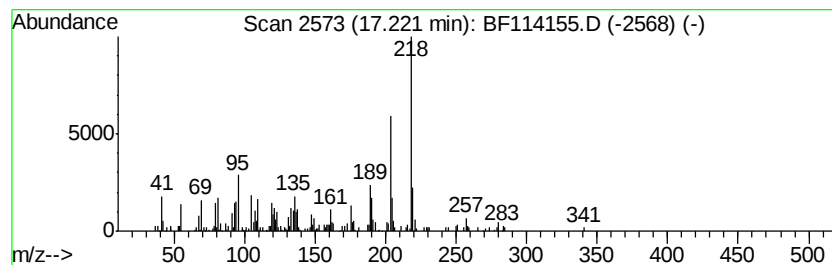
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Anthracene, 9-(2-propenyl)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.22	2.40 ng	261691	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	58
2		.alpha.-Amyrin, trimethylsilyl ether...	498	C33H58OSi	1000374-76-6	50
3		6H-[1,2]Dioxeto[3',4':4,5]furo[3,2-g][1]benzopyra...	260	C14H12O5	129812-24-4	50
4		Benzenamine, 2,6-dimethyl-N-(4,4-dimethyl-2,5-dihydro-2H-pyran-2-yl)-	218	C13H18N2O	281211-68-5	47
5		3a-Methyl-3,3a-dihydropyrrolo[3,2-b]pyridine	218	C11H10N2OS	017163-68-7	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051119\
Data File : BF114155.D
Acq On : 11 May 2019 14:28
Operator : JU/SJ
Sample : K2763-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P021-SS006-0002-01

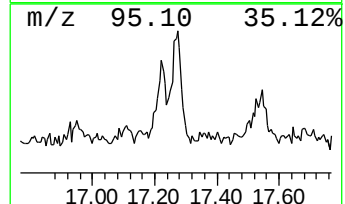
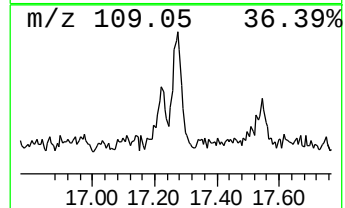
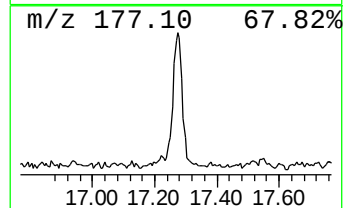
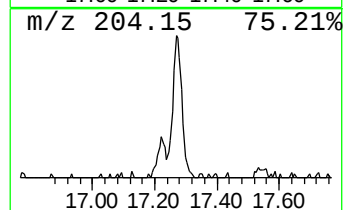
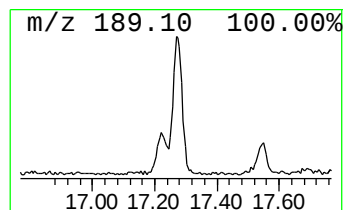
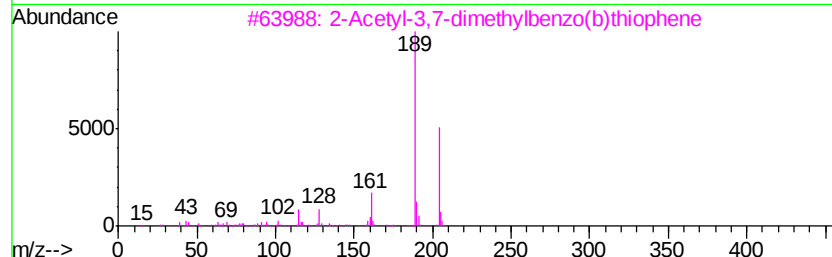
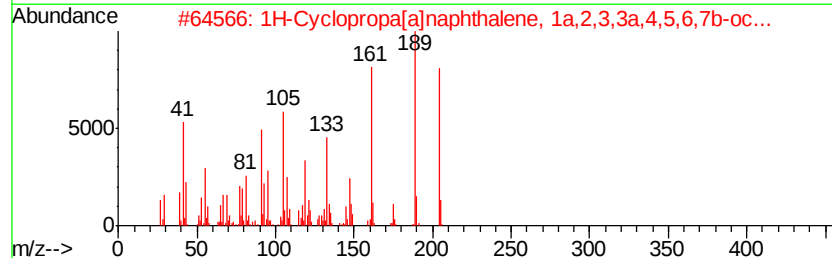
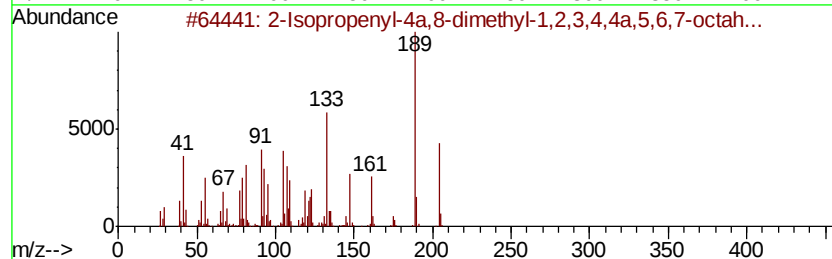
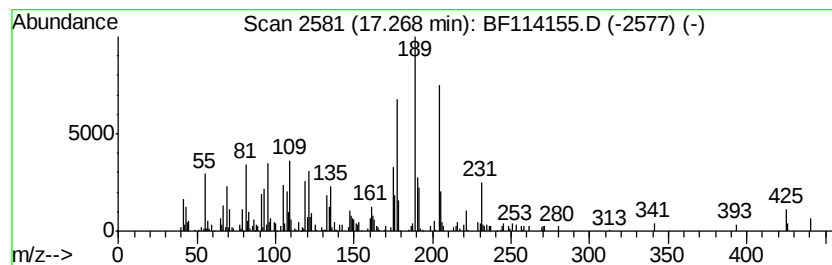
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.27 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.27	4.20 ng	458065	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	43
2		1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	38
3		2-Acetyl-3,7-dimethylbenzo(b)thi...	204	C12H12OS	006179-06-2	30
4		Benzene, 1,3,5-tris(1-methylethyl)-	204	C15H24	000717-74-8	27
5		1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051119\
 Data File : BF114155.D
 Acq On : 11 May 2019 14:28
 Operator : JU/SJ
 Sample : K2763-08
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P021-SS006-0002-01

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
Butane, 2-methoxy...	2.15	30.0	ng	2636900	1	6.85	1760390	20.0
unknown6.63	6.63	88.0	ng	7745580	1	6.85	1760390	20.0
n-Hexadecanoic acid	11.89	5.6	ng	801442	4	11.37	2875880	20.0
Octadecanoic acid	12.67	4.1	ng	595447	4	11.37	2875880	20.0
1-Hexadecanesulfo...	13.84	5.2	ng	530606	5	14.00	2048390	20.0
Octadecane	14.47	3.8	ng	384900	5	14.00	2048390	20.0
Tetracosane	14.78	4.1	ng	443612	6	15.47	2181880	20.0
Oxirane, heptadecyl-	14.92	2.0	ng	222180	6	15.47	2181880	20.0
Heptacosane	15.12	6.7	ng	733643	6	15.47	2181880	20.0
Heneicosane	16.43	4.2	ng	452277	6	15.47	2181880	20.0
Anthracene, 9-(2-...	17.22	2.4	ng	261691	6	15.47	2181880	20.0
unknown17.27	17.27	4.2	ng	458065	6	15.47	2181880	20.0