

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
 Data File : BF114138.D
 Acq On : 10 May 2019 23:13
 Operator : JU/SJ
 Sample : K2762-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P021-SS001-0206-01

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	2.128	3	7	14	rVB	1368572	1756426	31.12%	3.416%
2	5.075	505	508	512	rVB	49648	59734	1.06%	0.116%
3	5.481	573	577	591	rBV	5749935	5323786	94.32%	10.353%
4	6.487	744	748	759	rBV	5555040	5644300	100.00%	10.976%
5	6.628	768	772	775	rBV	5957983	5375920	95.25%	10.454%
6	6.851	807	810	814	rBV	2093355	1754024	31.08%	3.411%
7	7.010	833	837	840	rBV	4622693	3739235	66.25%	7.272%
8	7.410	901	905	908	rBV	3773643	3224535	57.13%	6.271%
9	8.134	1024	1028	1031	rBV	2545555	2081796	36.88%	4.048%
10	8.586	1102	1105	1115	rVB	71636	97895	1.73%	0.190%
11	9.204	1206	1210	1214	rBV	4957870	4086243	72.40%	7.946%
12	9.598	1273	1277	1281	rBV	795415	639489	11.33%	1.244%
13	9.792	1305	1310	1313	rBV2	44212	66753	1.18%	0.130%
14	9.886	1322	1326	1330	rVB	2410058	2024830	35.87%	3.938%
15	10.675	1455	1460	1463	rBV	2970979	2767599	49.03%	5.382%
16	11.369	1574	1578	1581	rBV	2360924	2081345	36.88%	4.048%
17	11.392	1581	1582	1585	rVB	179912	106523	1.89%	0.207%
18	11.898	1665	1668	1674	rBV	653862	610974	10.82%	1.188%
19	12.580	1781	1784	1789	rBV	247786	214616	3.80%	0.417%
20	12.680	1798	1801	1804	rBV2	257528	265982	4.71%	0.517%
21	12.810	1820	1823	1826	rBV	365232	296134	5.25%	0.576%
22	12.951	1843	1847	1850	rBV	4299676	3634324	64.39%	7.068%
23	13.851	1996	2000	2011	rBV2	345282	501448	8.88%	0.975%
24	14.004	2022	2026	2029	rBV	1897378	1897821	33.62%	3.691%
25	14.033	2029	2031	2033	rVB	114009	87591	1.55%	0.170%
26	14.168	2052	2054	2061	rVB	152958	149344	2.65%	0.290%
27	14.480	2104	2107	2111	rVB	271028	267376	4.74%	0.520%
28	14.786	2156	2159	2162	rVB	352002	305317	5.41%	0.594%
29	14.863	2169	2172	2176	rVB	218165	227165	4.02%	0.442%
30	15.121	2213	2216	2219	rBV	411581	440864	7.81%	0.857%
31	15.474	2272	2276	2279	rBV	1086000	1421110	25.18%	2.764%
32	15.933	2351	2354	2359	rVB	204277	272180	4.82%	0.529%

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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P021-SS001-0206-01

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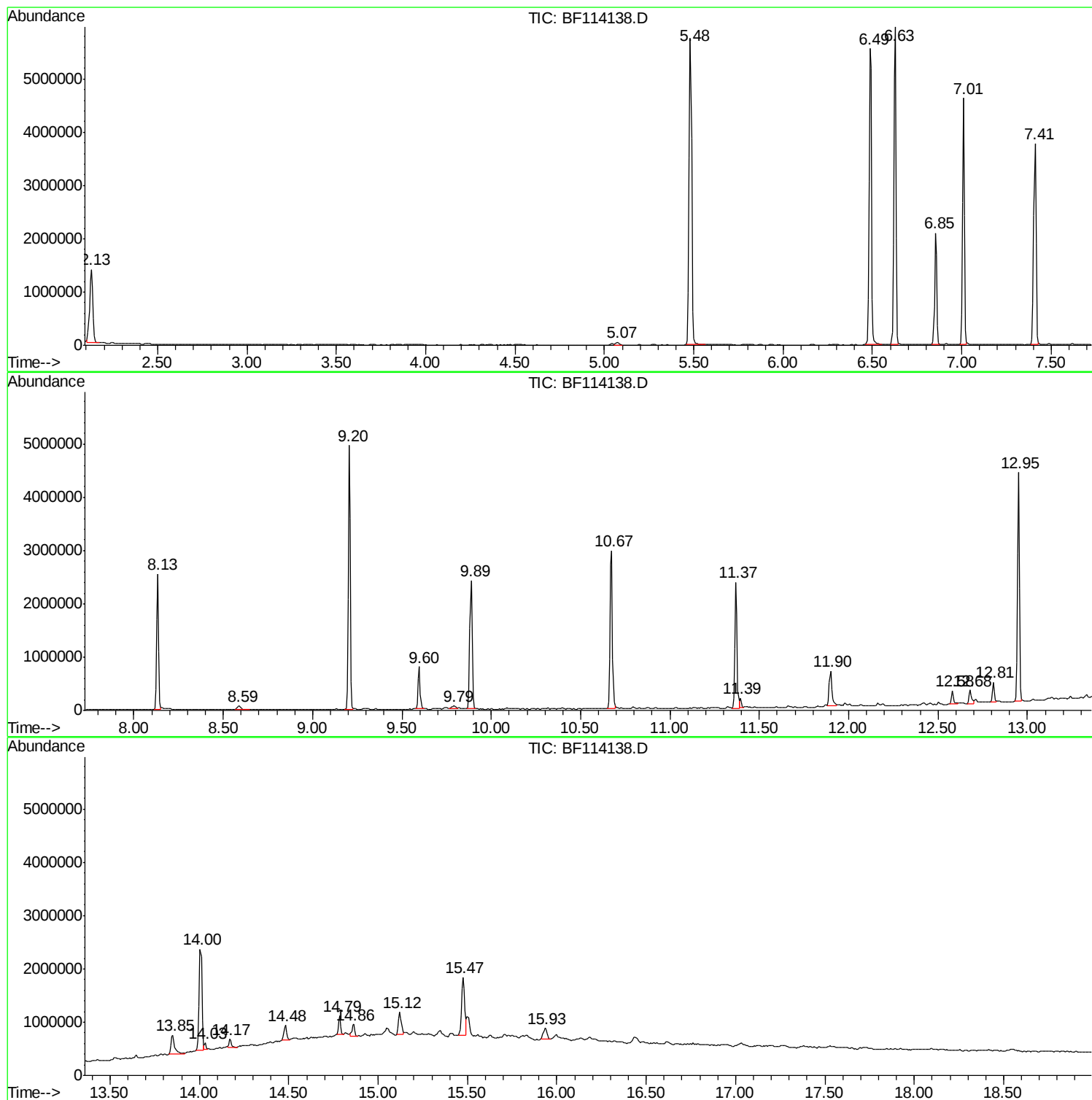
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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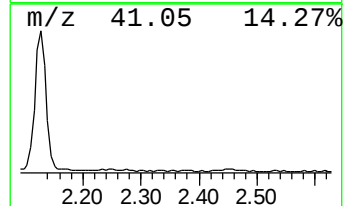
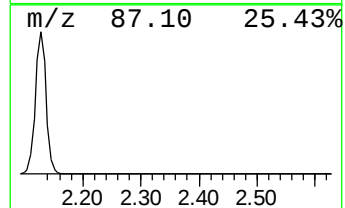
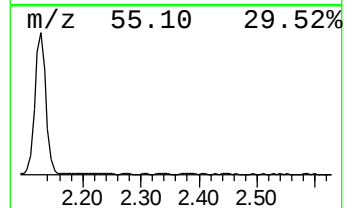
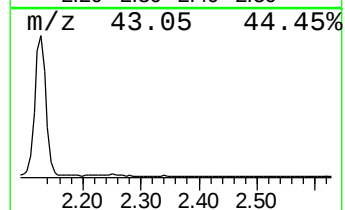
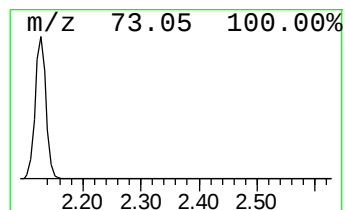
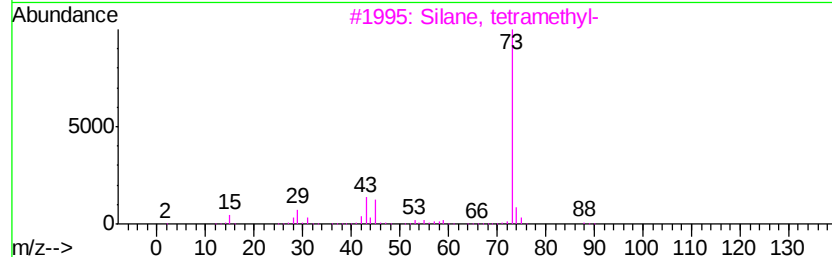
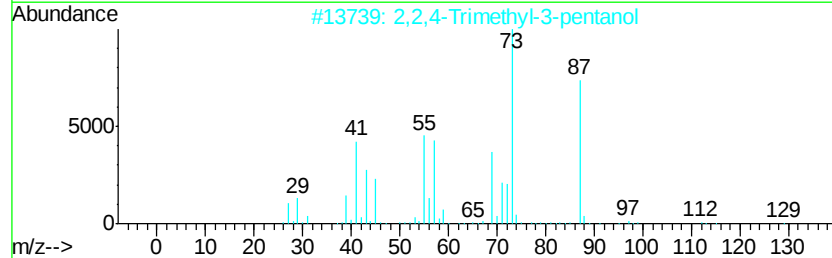
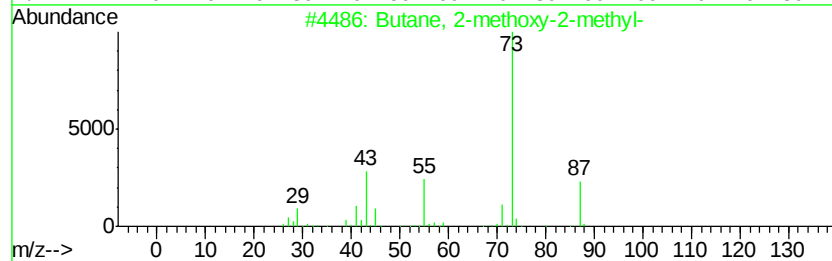
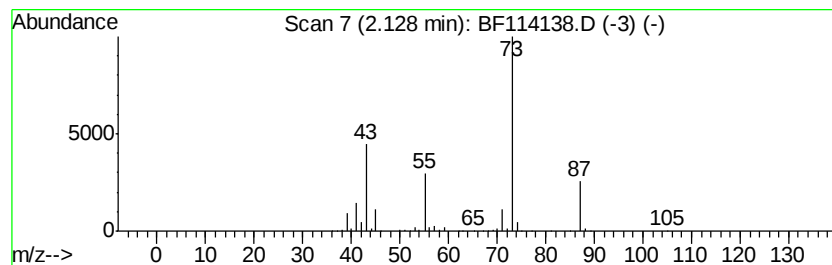
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.13	20.03 ng	1756430	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	40
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	23



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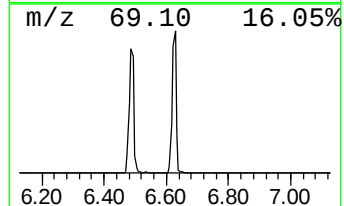
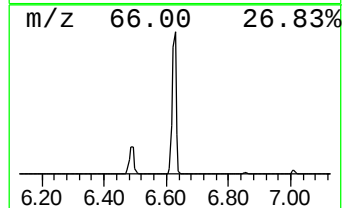
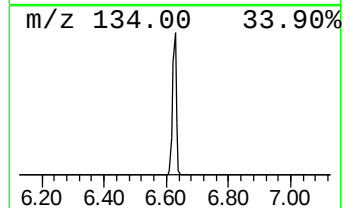
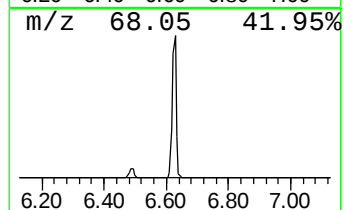
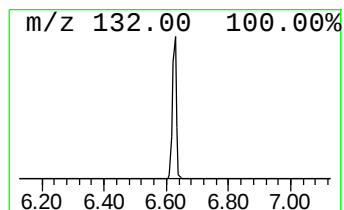
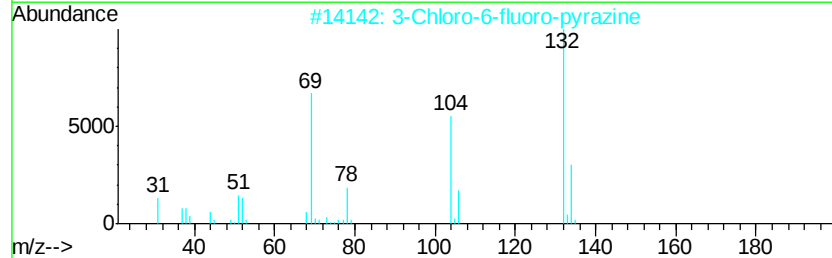
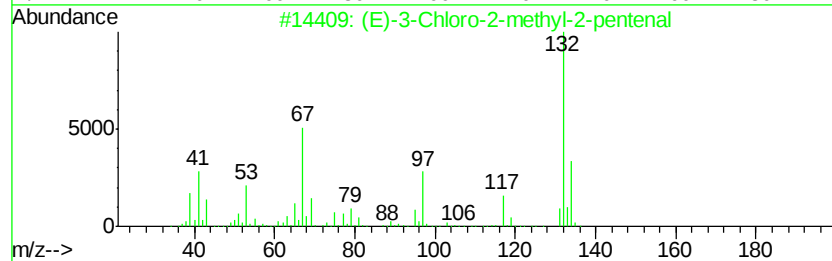
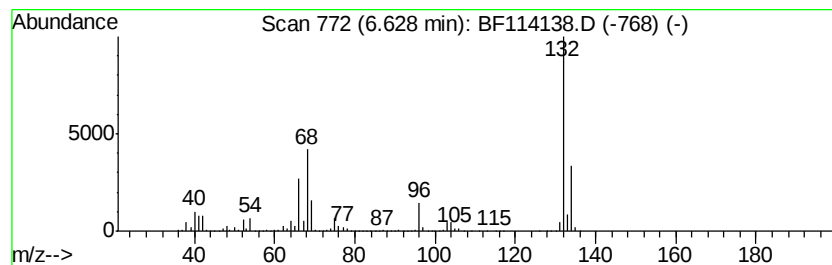
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	61.30 ng	5375920	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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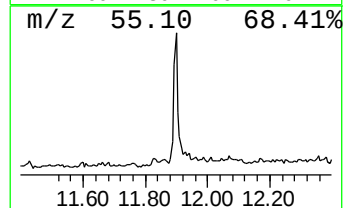
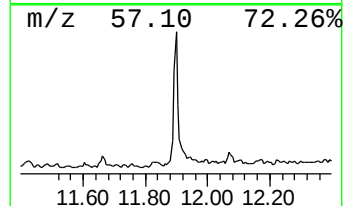
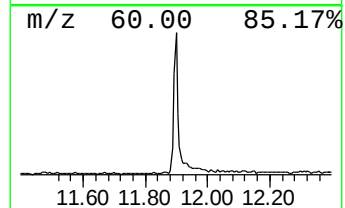
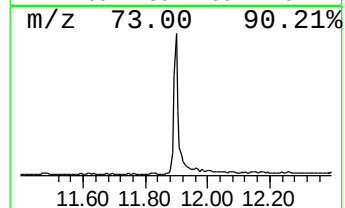
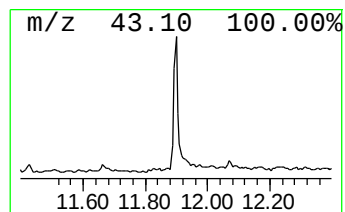
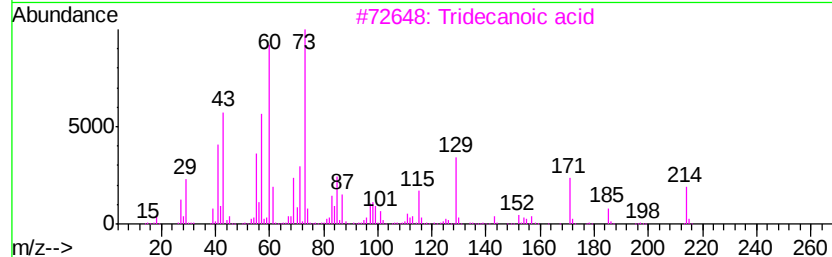
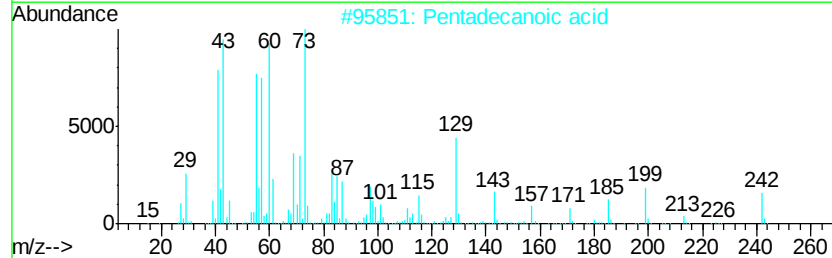
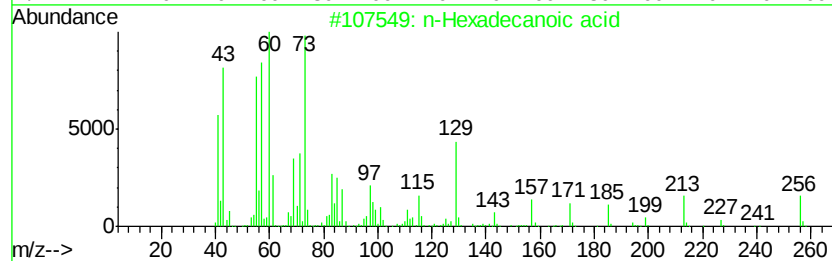
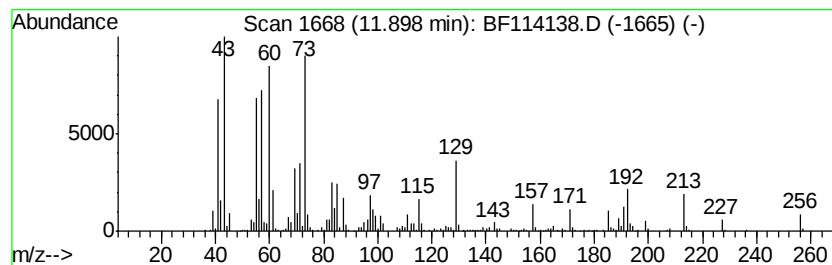
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.90	5.87 ng	610974	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	70
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53



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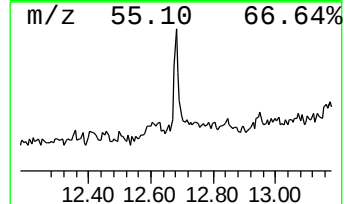
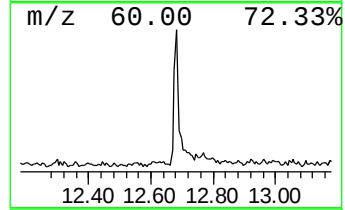
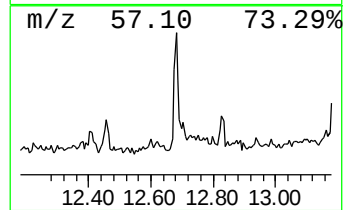
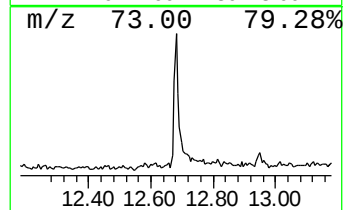
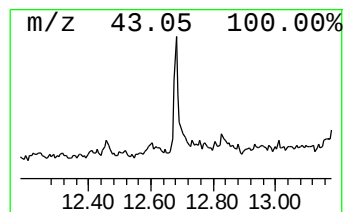
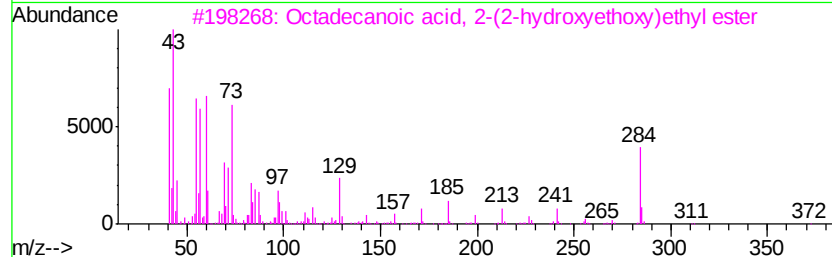
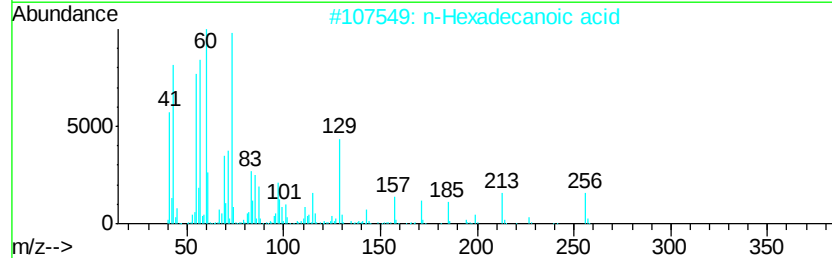
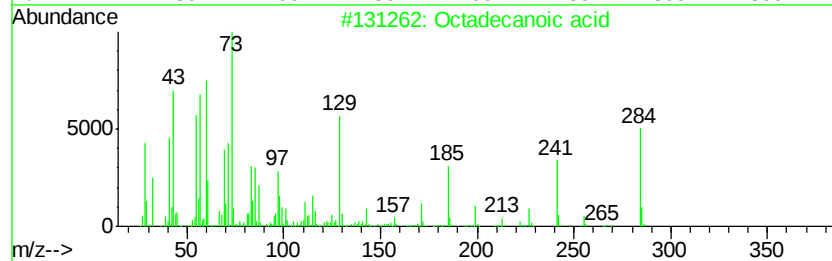
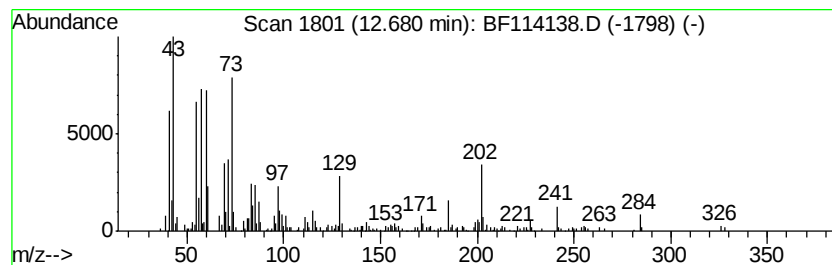
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	2.56 ng	265982	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	78
5		Undecanoic acid	186	C11H22O2	000112-37-8	60



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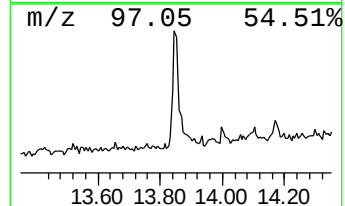
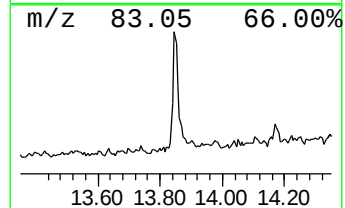
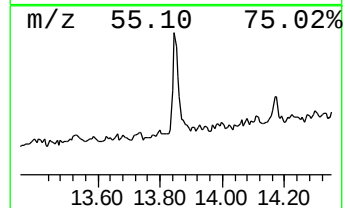
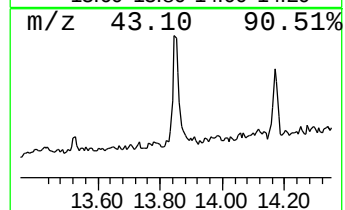
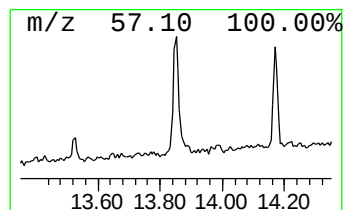
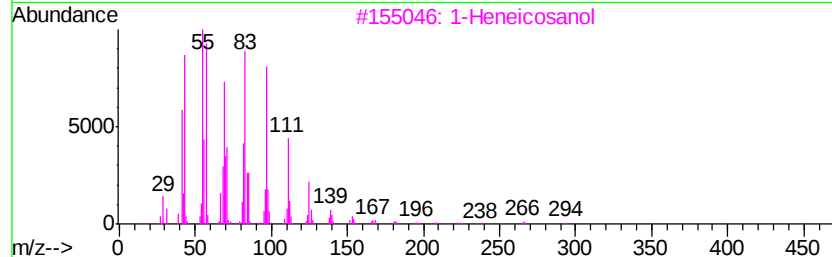
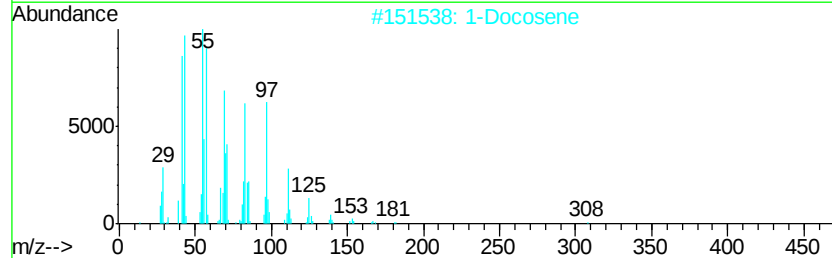
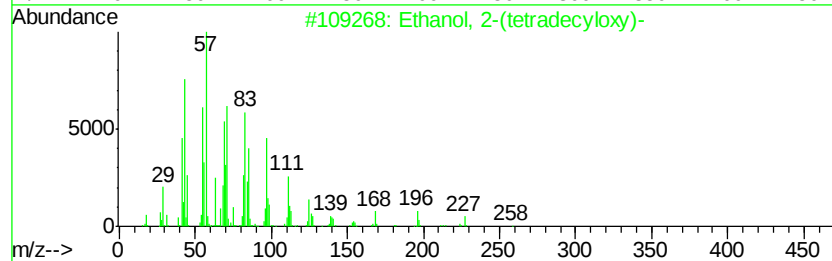
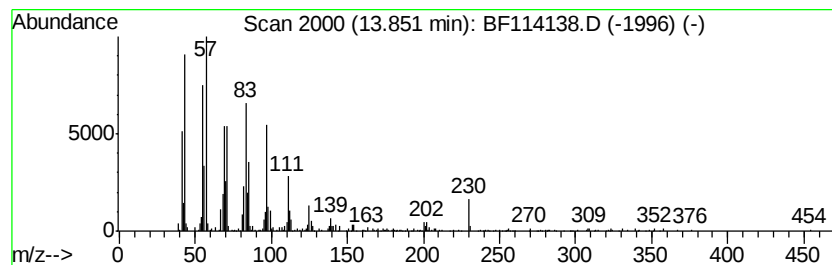
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.85	5.28 ng	501448	Chrysene-d12	14.00	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	99
2	1-Docosene	308	C22H44	001599-67-3	99
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91



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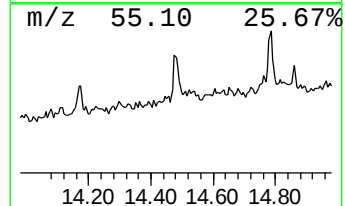
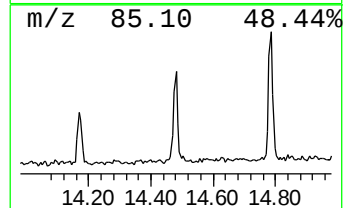
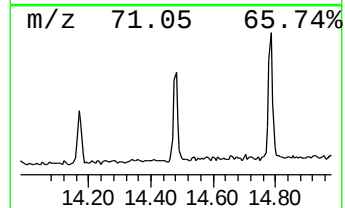
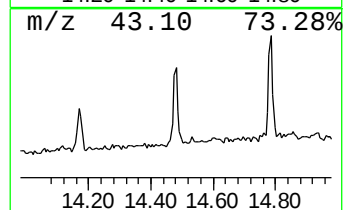
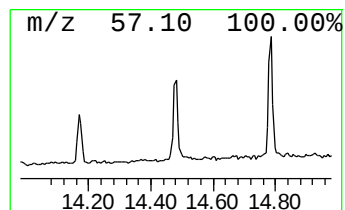
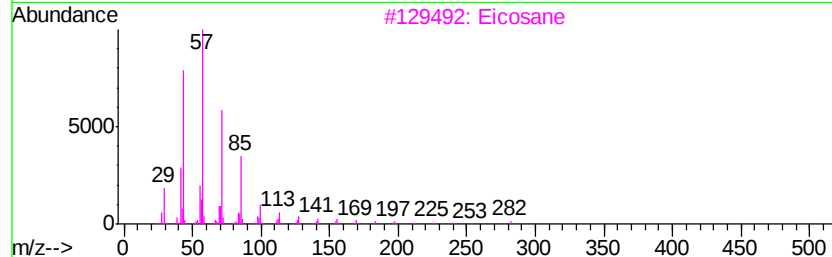
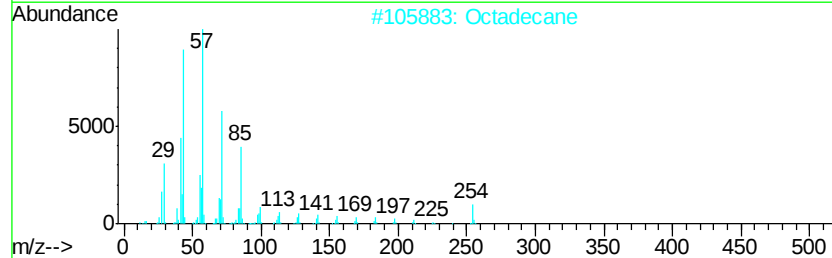
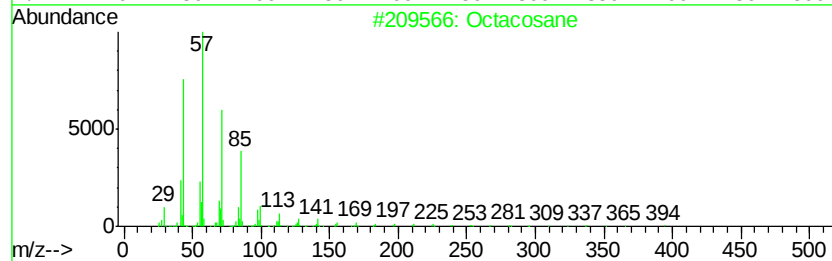
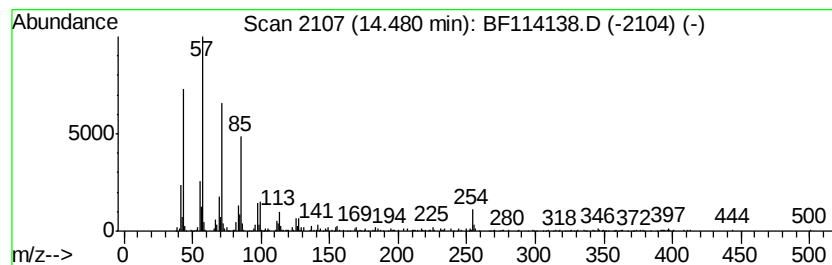
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	2.82 ng	267376	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	94
2		Octadecane	254	C18H38	000593-45-3	87
3		Eicosane	282	C20H42	000112-95-8	80
4		Nonadecane	268	C19H40	000629-92-5	80
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
Data File : BF114138.D
Acq On : 10 May 2019 23:13
Operator : JU/SJ
Sample : K2762-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P021-SS001-0206-01

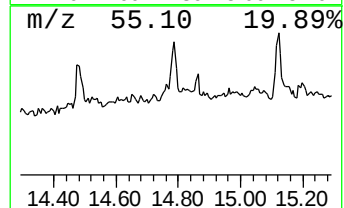
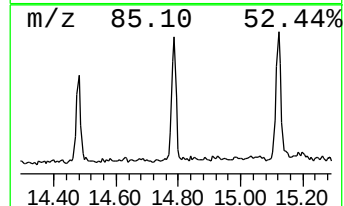
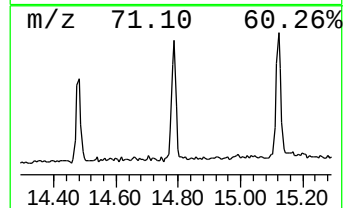
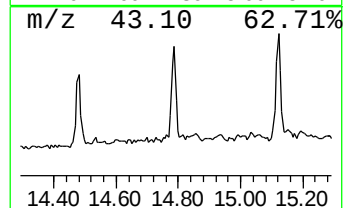
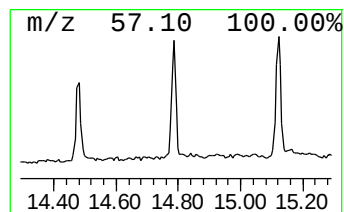
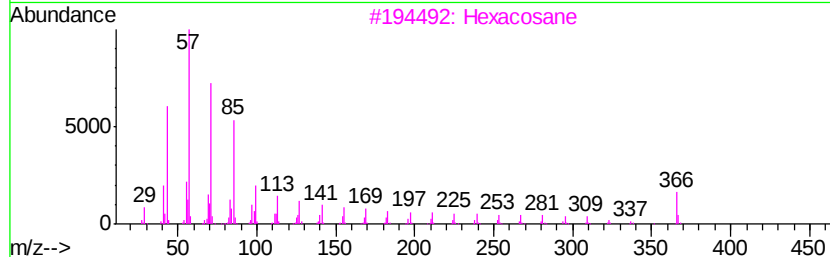
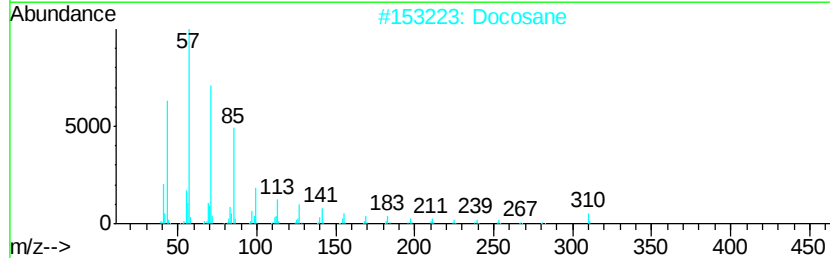
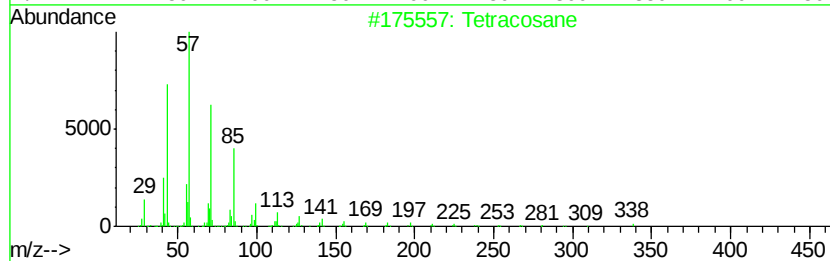
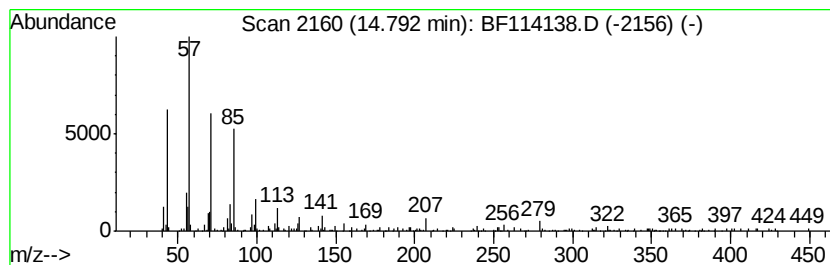
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	4.30 ng	305317	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	93
2		Docosane	310	C22H46	000629-97-0	93
3		Hexacosane	366	C26H54	000630-01-3	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Tricosane, 2-methyl-	338	C24H50	001928-30-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
Data File : BF114138.D
Acq On : 10 May 2019 23:13
Operator : JU/SJ
Sample : K2762-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P021-SS001-0206-01

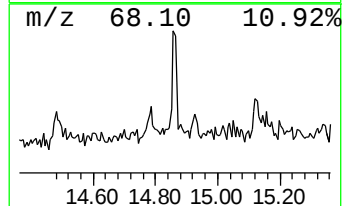
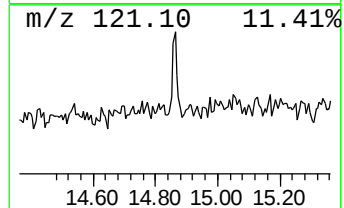
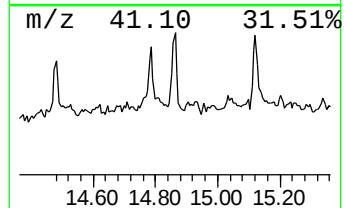
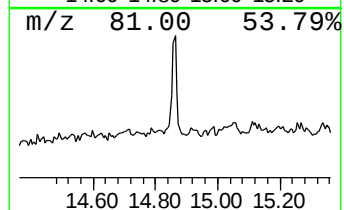
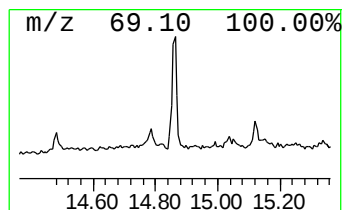
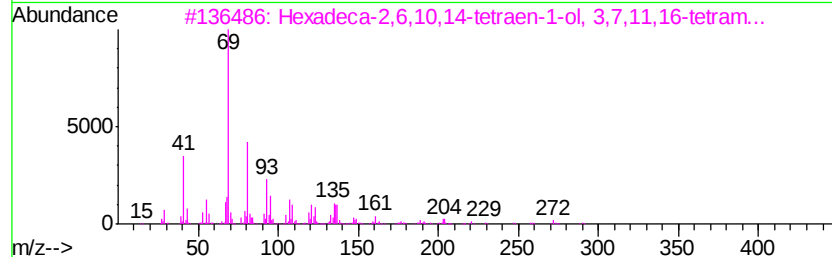
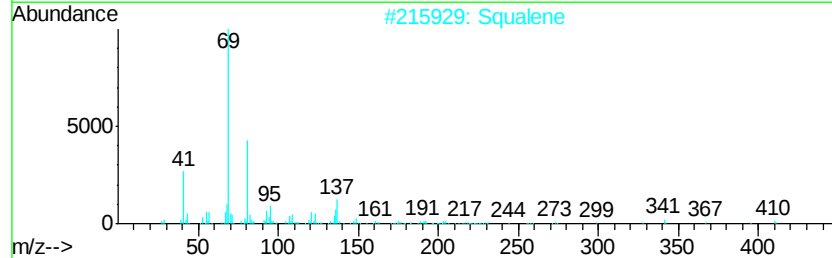
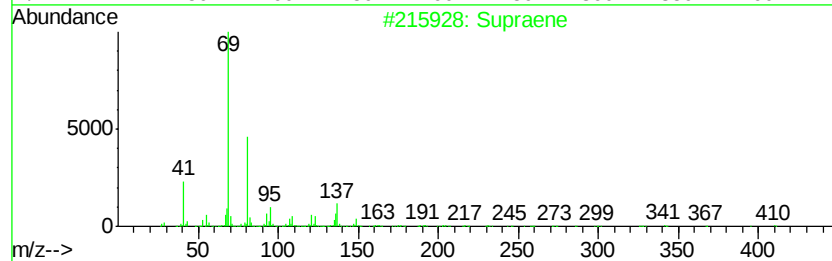
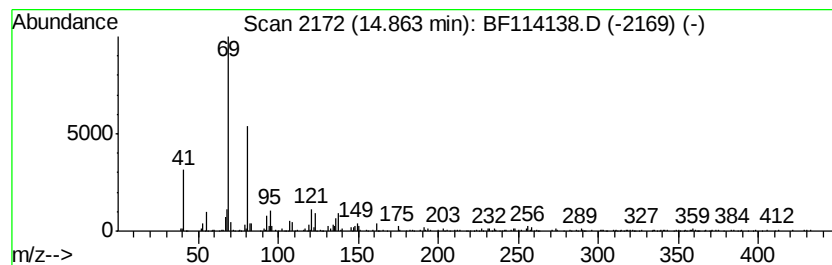
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	3.20 ng	227165	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	72
2		Squalene	410	C30H50	000111-02-4	64
3		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	64
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	56
5		2-Propenoic acid, 2-methyl-, 2-p...	124	C7H8O2	013861-22-8	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
Data File : BF114138.D
Acq On : 10 May 2019 23:13
Operator : JU/SJ
Sample : K2762-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

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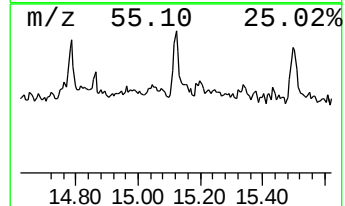
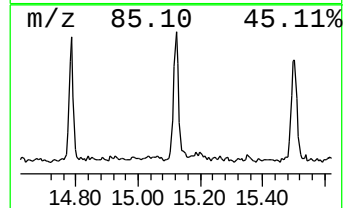
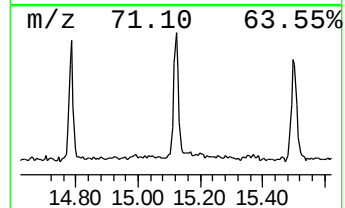
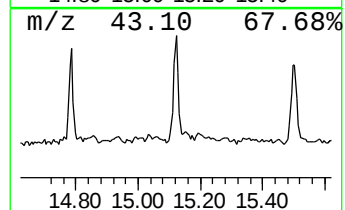
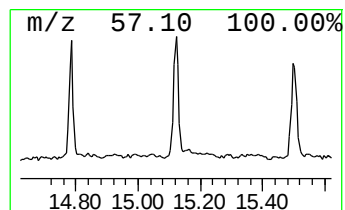
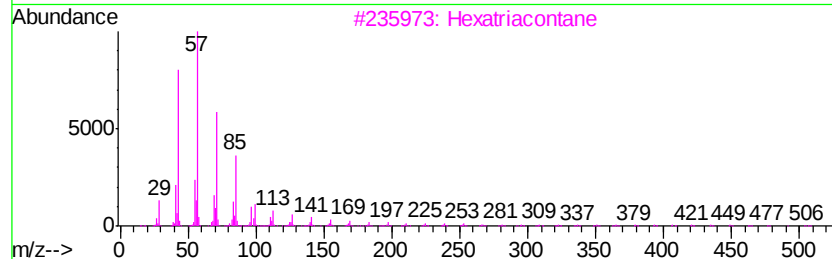
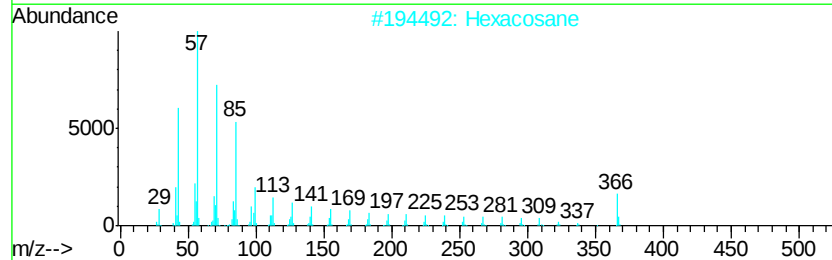
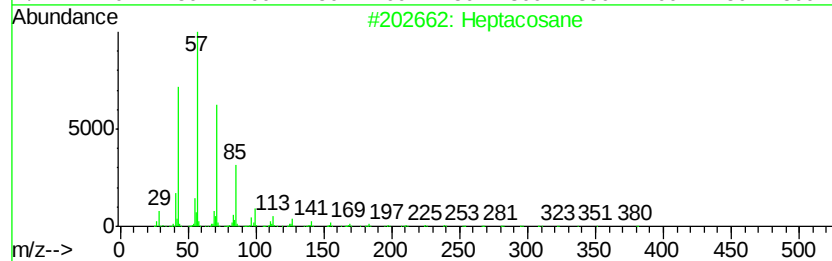
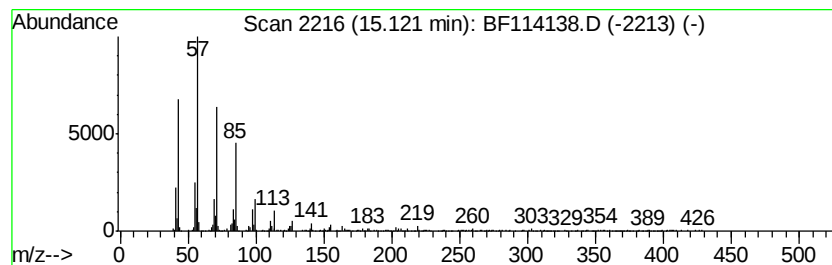
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	6.20 ng	440864	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	96
2		Hexacosane	366	C26H54	000630-01-3	90
3		Hexatriacontane	507	C36H74	000630-06-8	87
4		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
5		Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051019\
Data File : BF114138.D
Acq On : 10 May 2019 23:13
Operator : JU/SJ
Sample : K2762-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P021-SS001-0206-01

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.63	6.63	61.3	ng	5375920	1	6.85	1754020	20.0
n-Hexadecanoic acid	11.90	5.9	ng	610974	4	11.37	2081350	20.0
Octadecanoic acid	12.68	2.6	ng	265982	4	11.37	2081350	20.0
Ethanol, 2-(tetra...	13.85	5.3	ng	501448	5	14.00	1897820	20.0
Octacosane	14.48	2.8	ng	267376	5	14.00	1897820	20.0
Tetracosane	14.79	4.3	ng	305317	6	15.47	1421110	20.0
Supraene	14.86	3.2	ng	227165	6	15.47	1421110	20.0
Heptacosane	15.12	6.2	ng	440864	6	15.47	1421110	20.0