

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG101518\
 Data File : BG037336.D
 Acq On : 15 Oct 2018 16:45
 Operator : JU/SJ
 Sample : J5509-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

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_G\METHODS\8270-BG101118.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

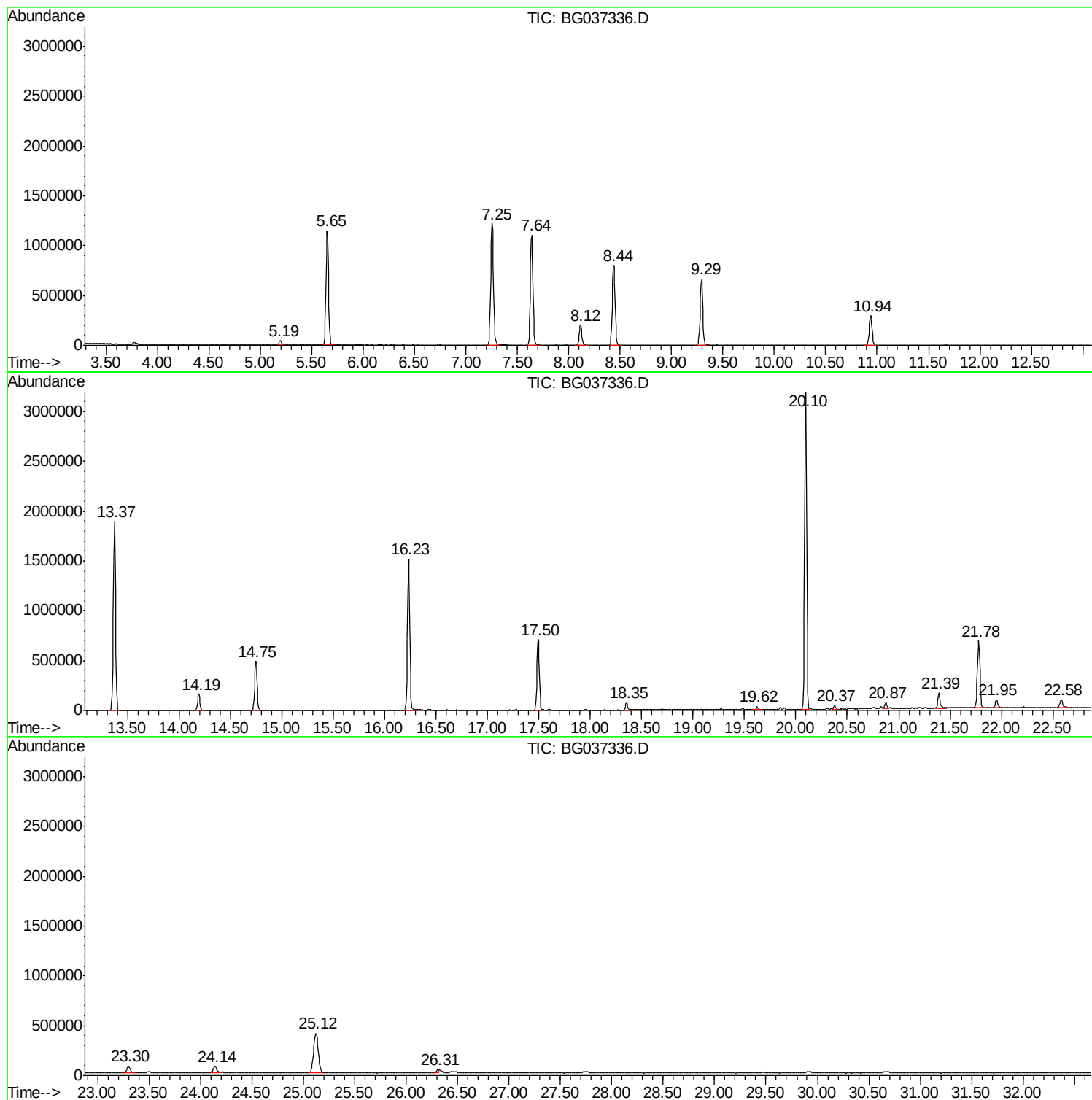
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.192	319	324	332	rBV	44050	72537	1.62%	0.285%
2	5.650	395	402	413	rBV	1150123	1882148	42.02%	7.403%
3	7.254	667	675	687	rBV	1222242	2221992	49.60%	8.740%
4	7.642	733	741	754	rBV	1106769	1964398	43.85%	7.727%
5	8.118	812	822	833	rVB	199748	365819	8.17%	1.439%
6	8.435	869	876	887	rVB	801131	1466568	32.74%	5.769%
7	9.293	1014	1022	1032	rBV	666817	1221522	27.27%	4.805%
8	10.938	1292	1302	1310	rBV	294837	545351	12.17%	2.145%
9	13.371	1708	1716	1724	rBV	1899732	3098664	69.17%	12.188%
10	14.193	1849	1856	1862	rBV	163341	240293	5.36%	0.945%
11	14.745	1943	1950	1958	rBV2	493145	830029	18.53%	3.265%
12	16.232	2196	2203	2220	rBV	1518467	2320359	51.80%	9.127%
13	17.495	2409	2418	2425	rBV2	706814	1118250	24.96%	4.399%
14	18.353	2559	2564	2574	rBV2	74947	118715	2.65%	0.467%
15	19.622	2772	2780	2787	rBV4	30838	49730	1.11%	0.196%
16	20.098	2854	2861	2867	rBV	3184028	4479463	100.00%	17.620%
17	20.374	2904	2908	2913	rVB	35222	46062	1.03%	0.181%
18	20.873	2989	2993	2997	rBV	57593	70946	1.58%	0.279%
19	21.391	3075	3081	3094	rBV	154349	255289	5.70%	1.004%
20	21.778	3138	3147	3158	rBV	675676	1172728	26.18%	4.613%
21	21.949	3171	3176	3186	rVB	78468	130724	2.92%	0.514%
22	22.577	3278	3283	3295	rBV2	78288	165496	3.69%	0.651%
23	23.300	3399	3406	3415	rBV3	70127	144821	3.23%	0.570%
24	24.140	3542	3549	3558	rBV	64596	152315	3.40%	0.599%
25	25.121	3705	3716	3727	rBV3	397347	1224980	27.35%	4.818%
26	26.314	3911	3919	3920	rBV7	33416	63988	1.43%	0.252%

Sum of corrected areas: 25423187

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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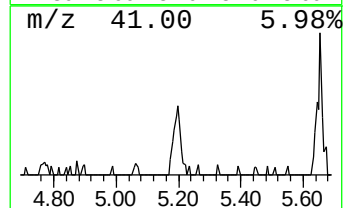
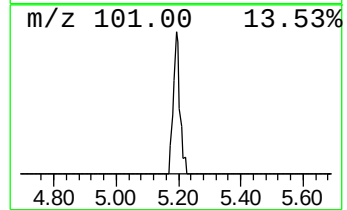
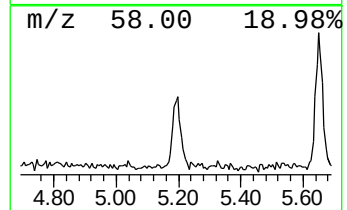
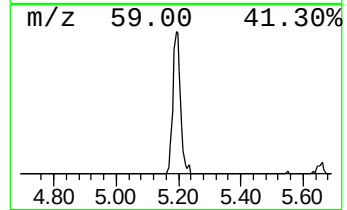
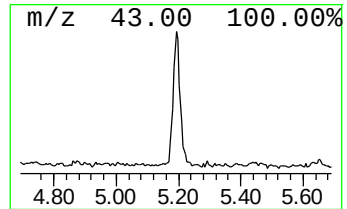
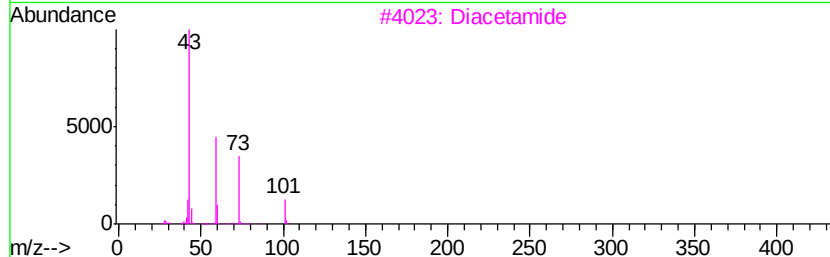
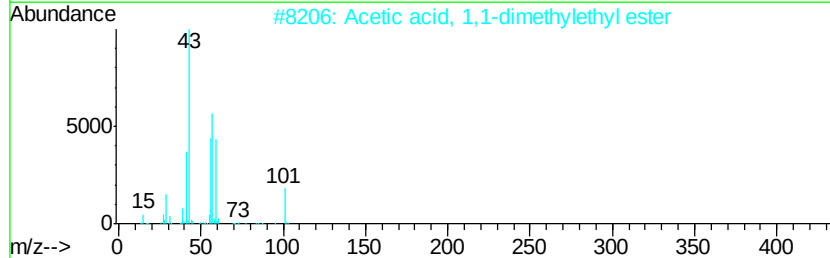
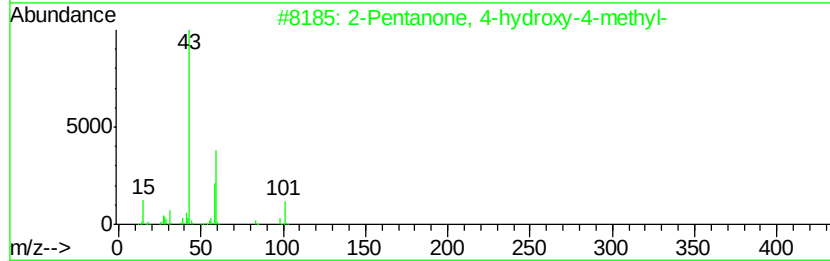
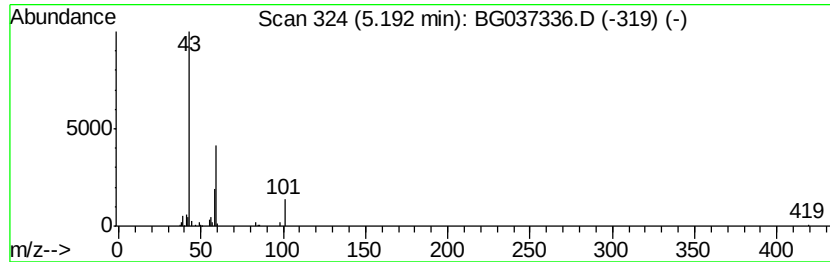
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.97 ng	72537	1,4-Dichlorobenzene-d4	8.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Diacetamide	101	C4H7NO2	000625-77-4	9
4			1-Ethoxypropan-2-yl acetate	146	C7H14O3	1000378-33-2	9
5			2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9



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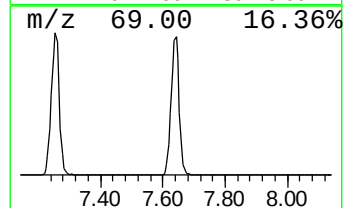
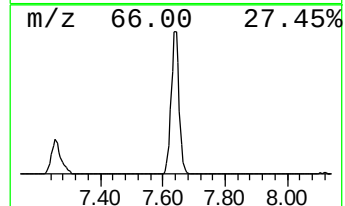
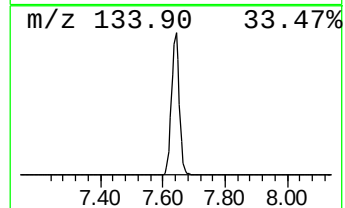
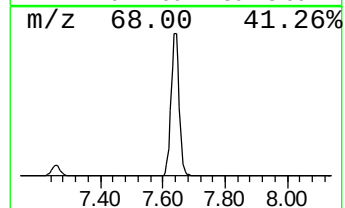
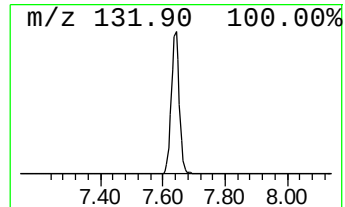
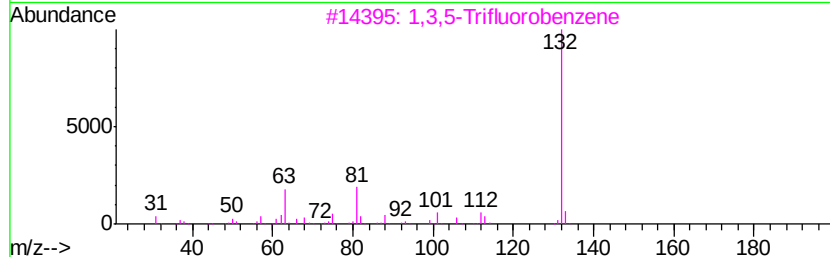
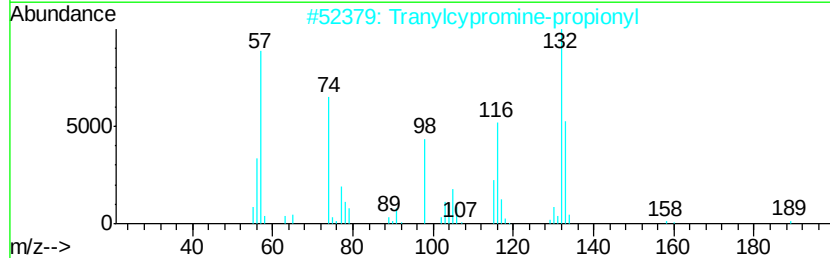
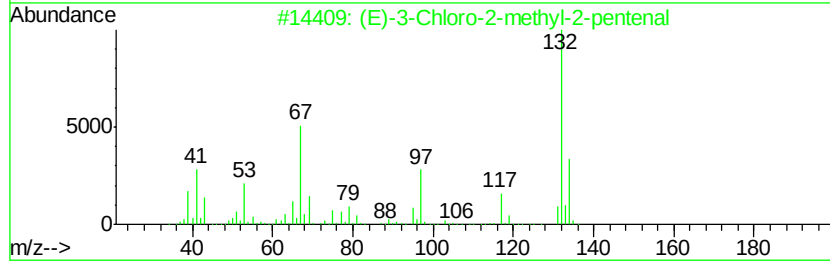
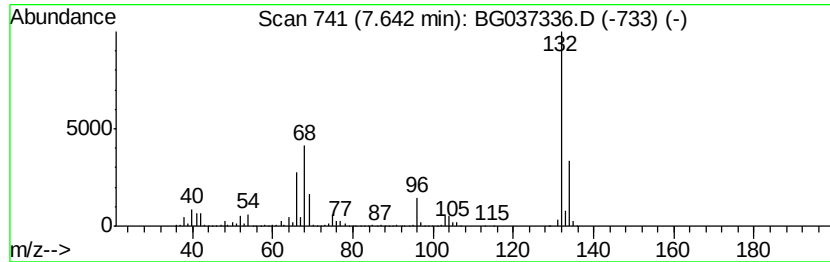
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	107.40 ng	1964400	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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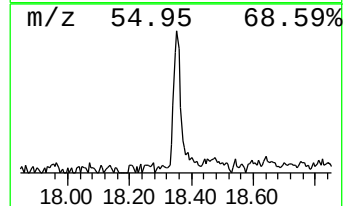
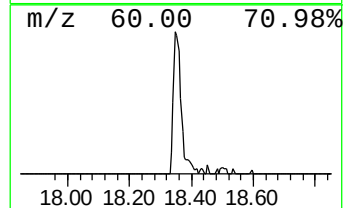
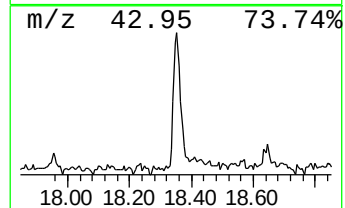
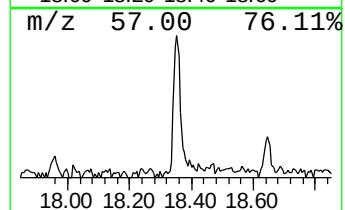
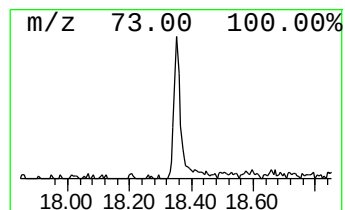
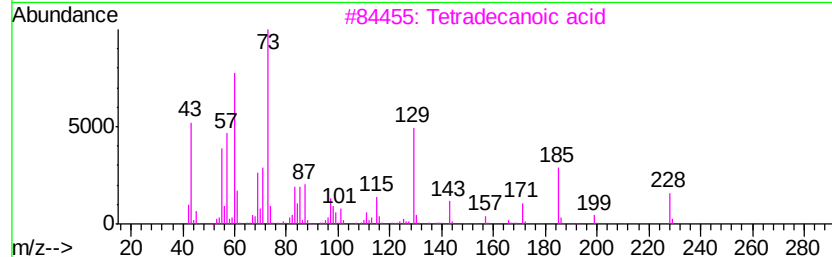
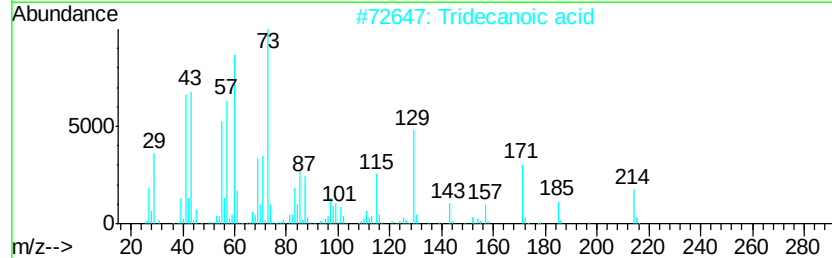
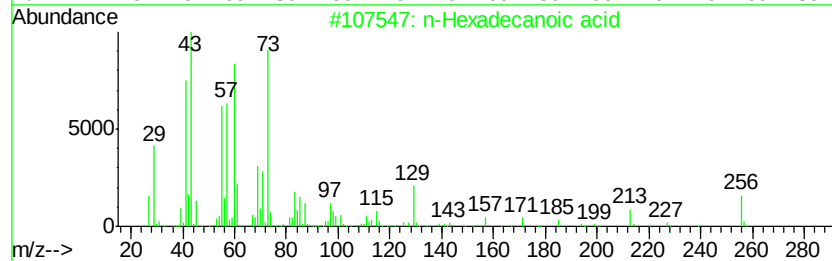
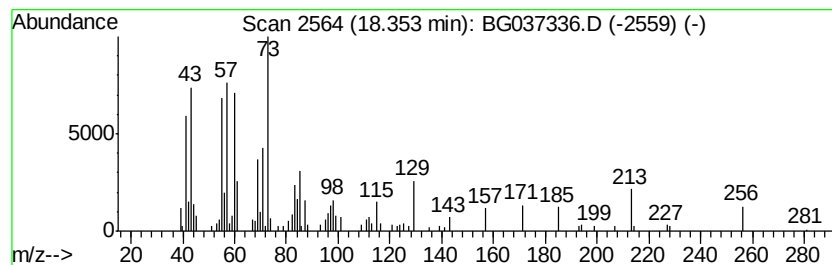
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.35	2.12 ng	118715	Phenanthrene-d10	17.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	60
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18
5		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	18



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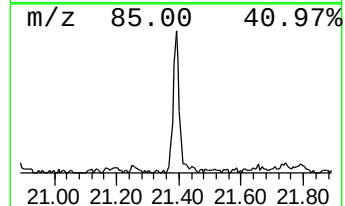
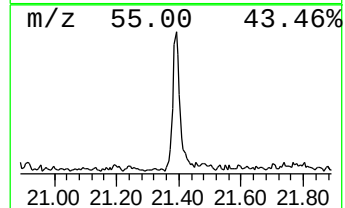
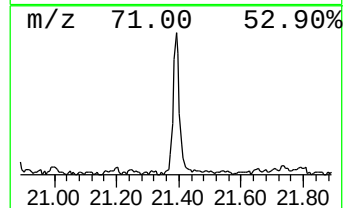
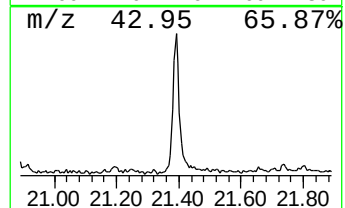
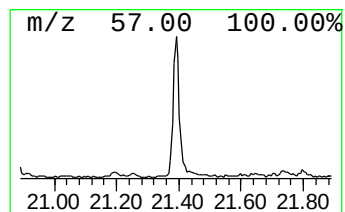
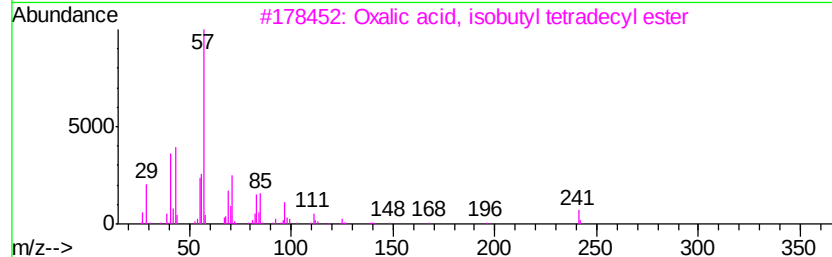
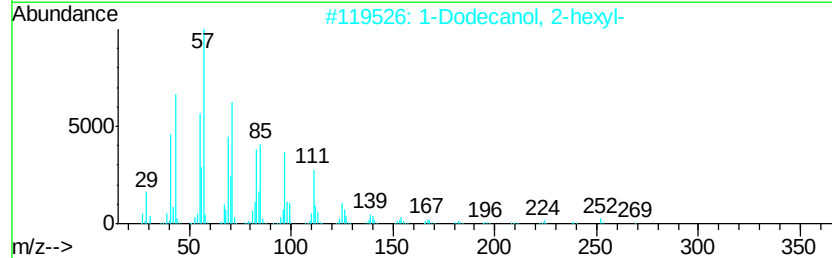
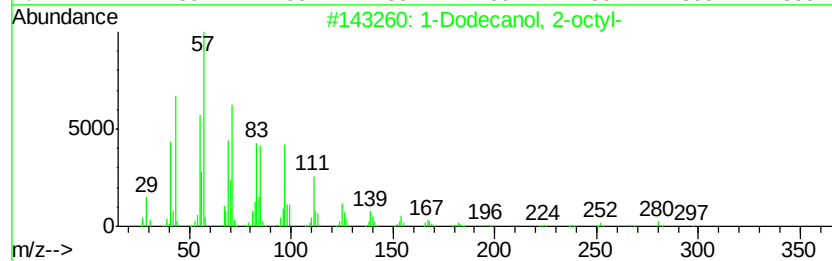
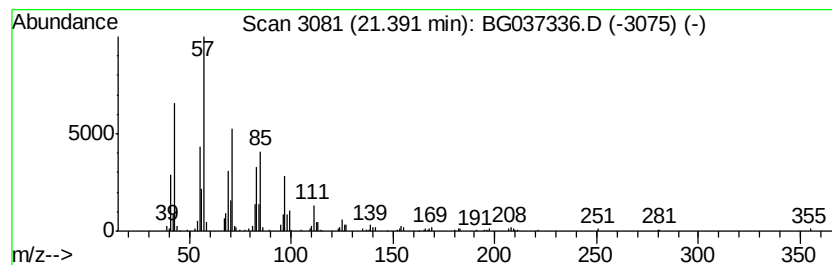
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Peak Number 5 1-Dodecanol, 2-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.39	4.35 ng	255289	Chrysene-d12	21.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
2		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	83
3		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	83
4		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	83
5		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	83



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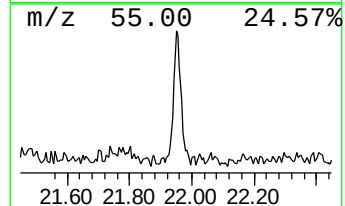
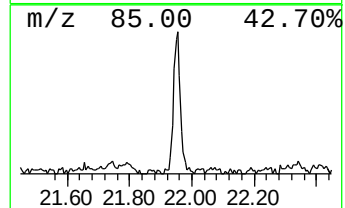
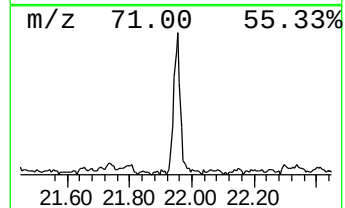
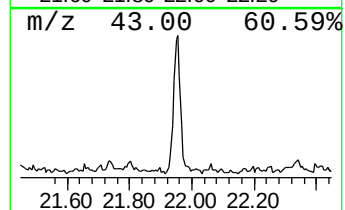
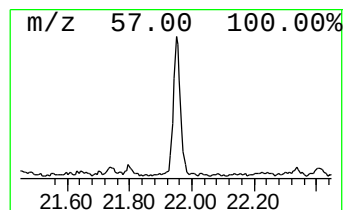
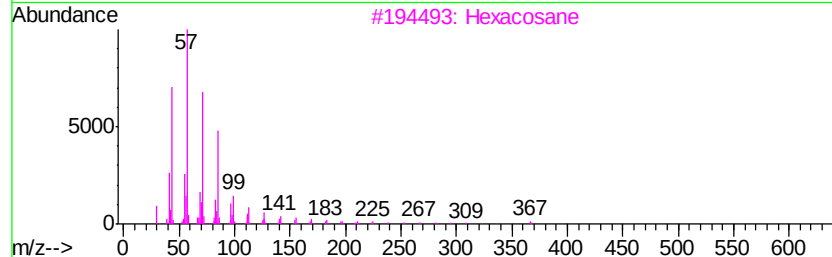
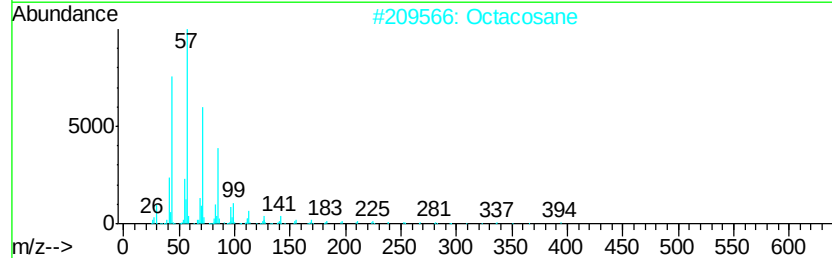
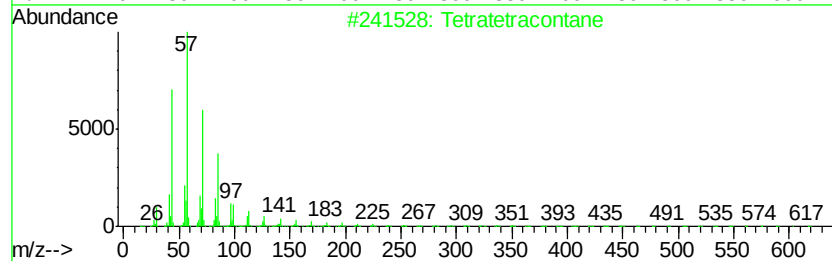
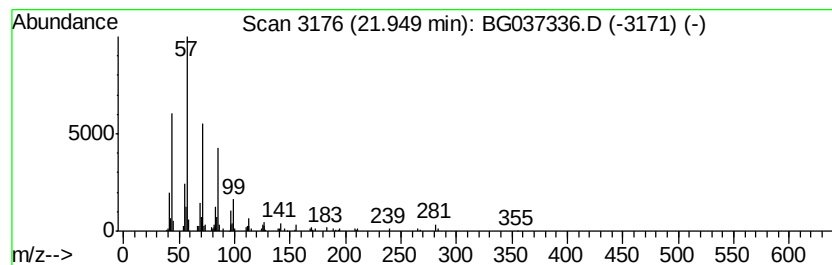
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Peak Number 6 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.95	2.23 ng	130724	Chrysene-d12	21.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Hexacosane	366	C26H54	000630-01-3	87
4		Nonadecane	268	C19H40	000629-92-5	83
5		Heneicosane	296	C21H44	000629-94-7	81



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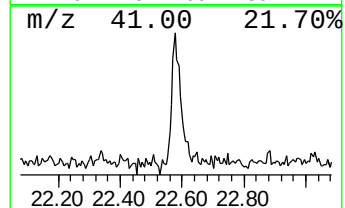
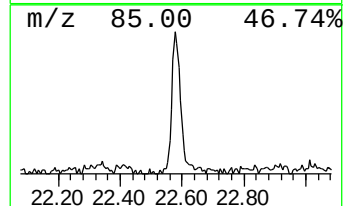
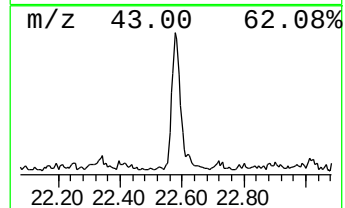
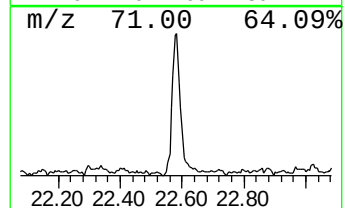
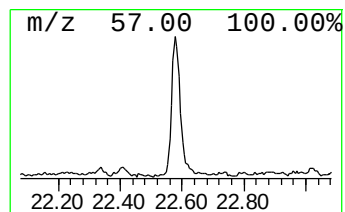
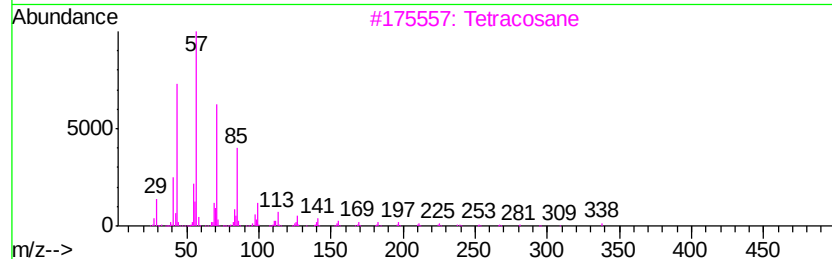
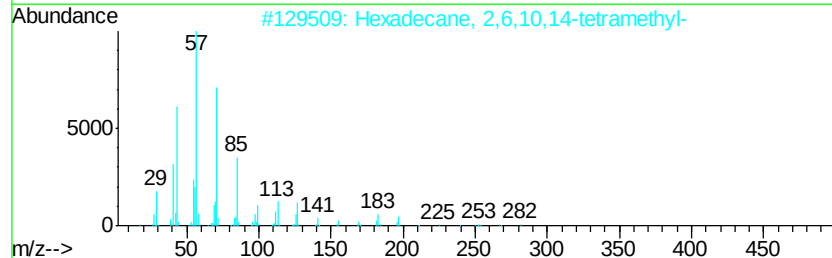
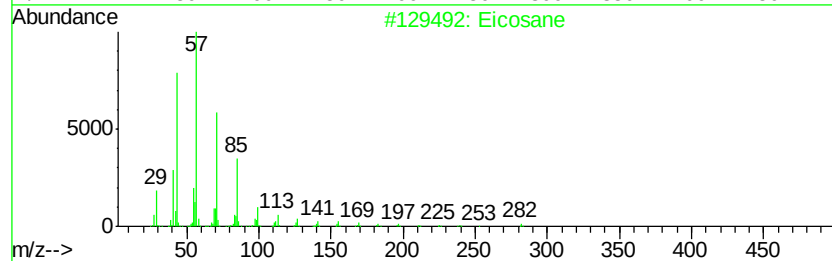
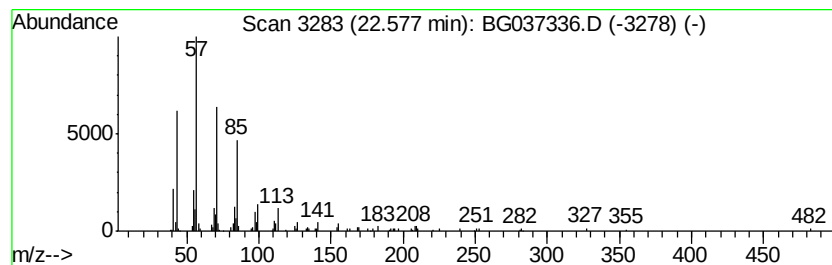
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.58	2.82 ng	165496	Chrysene-d12	21.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
3		Tetracosane	338	C24H50	000646-31-1	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG101518\
Data File : BG037336.D
Acq On : 15 Oct 2018 16:45
Operator : JU/SJ
Sample : J5509-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

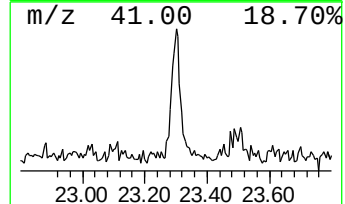
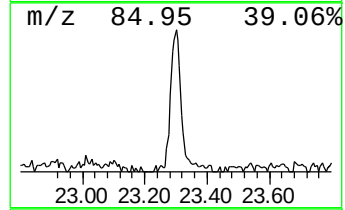
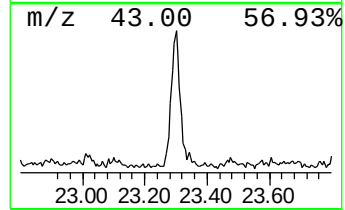
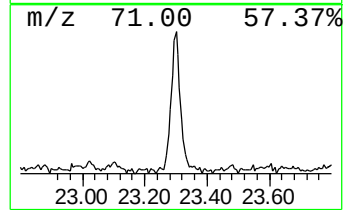
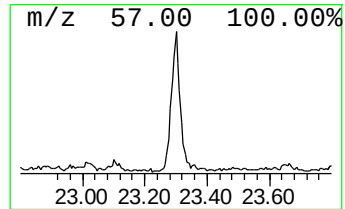
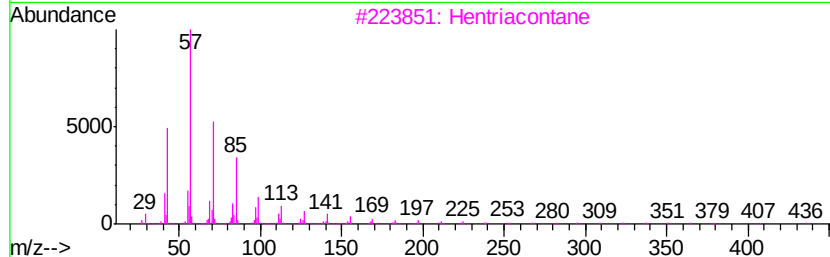
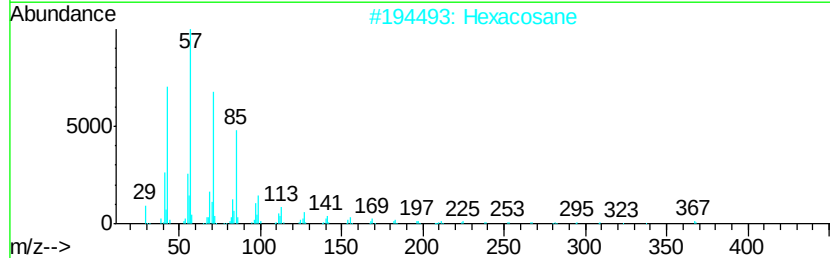
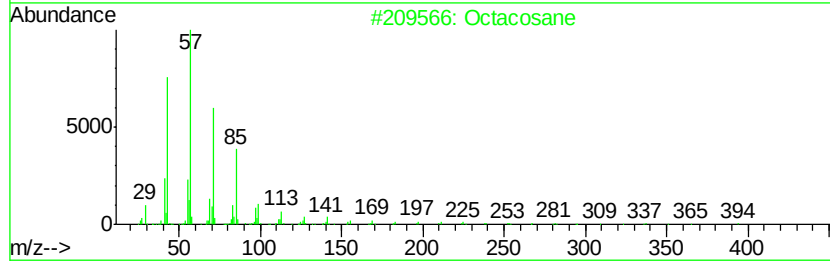
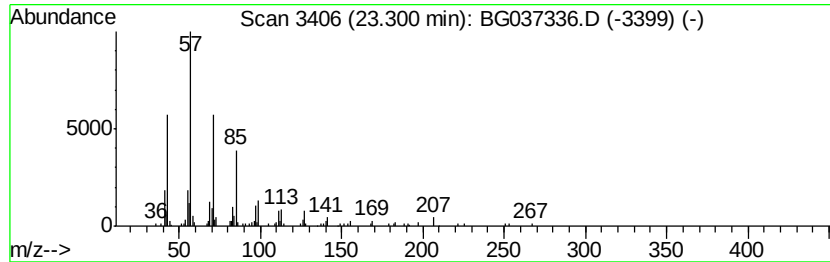
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	2.47 ng	144821	Chrysene-d12	21.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	90
2	Hexacosane		366	C26H54	000630-01-3	90
3	Hentriacontane		437	C31H64	000630-04-6	90
4	Heptacosane		380	C27H56	000593-49-7	87
5	Heneicosane		296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG101518\
Data File : BG037336.D
Acq On : 15 Oct 2018 16:45
Operator : JU/SJ
Sample : J5509-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

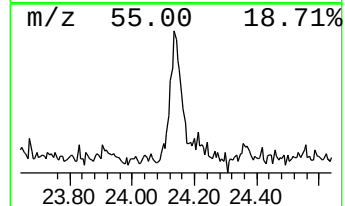
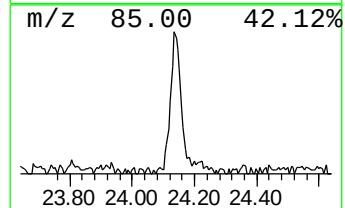
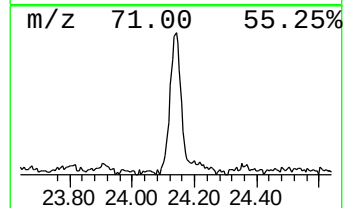
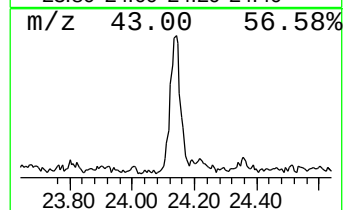
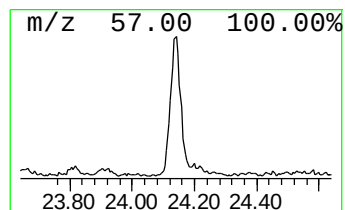
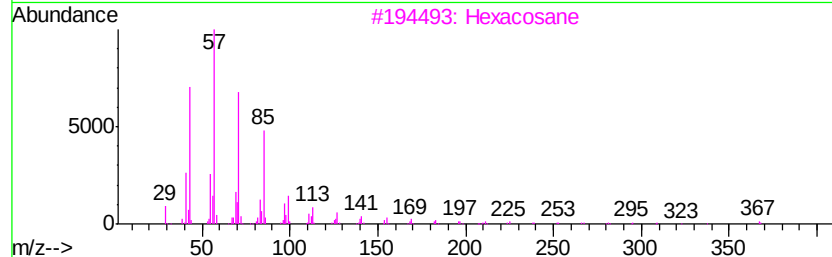
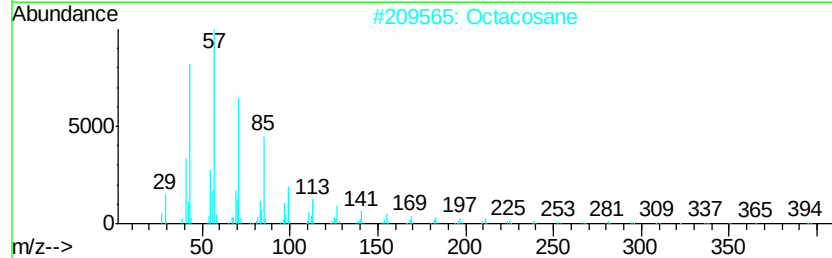
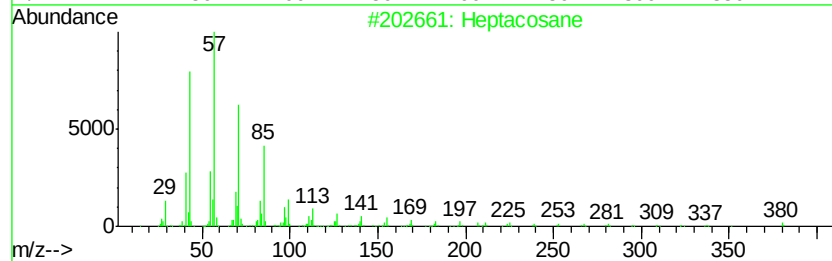
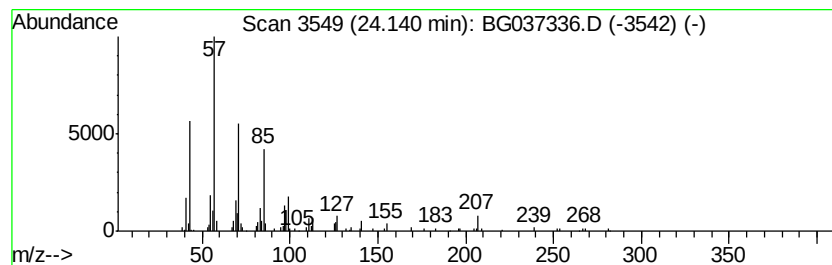
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
24.14	2.49 ng	152315	Perylene-d12	25.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	90
2	Octacosane		394	C28H58	000630-02-4	86
3	Hexacosane		366	C26H54	000630-01-3	81
4	Hexatriacontane		507	C36H74	000630-06-8	76
5	Octadecane		254	C18H38	000593-45-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG101518\
Data File : BG037336.D
Acq On : 15 Oct 2018 16:45
Operator : JU/SJ
Sample : J5509-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.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...	5.19	4.0	ng	72537	1	8.12	365819	20.0
unknown7.64	7.64	107.4	ng	1964400	1	8.12	365819	20.0
n-Hexadecanoic acid	18.35	2.1	ng	118715	4	17.49	1118250	20.0
1-Dodecanol, 2-oc...	21.39	4.3	ng	255289	5	21.78	1172730	20.0
Tetratetracontane	21.95	2.2	ng	130724	5	21.78	1172730	20.0
Eicosane	22.58	2.8	ng	165496	5	21.78	1172730	20.0
Octacosane	23.30	2.5	ng	144821	5	21.78	1172730	20.0
Heptacosane	24.14	2.5	ng	152315	6	25.12	1224980	20.0