

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020819\
 Data File : BG039423.D
 Acq On : 8 Feb 2019 19:54
 Operator : JU/SJ
 Sample : K1404-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A0C12-SS4-10.0-10.5

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_G\METHODS\8270-BG012919.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	3.223	17	23	32	rBV	79444	150481	3.69%	0.569%
2	3.299	32	36	42	rVB	58659	84017	2.06%	0.318%
3	5.256	363	369	376	rBV	80985	128006	3.14%	0.484%
4	5.714	440	447	455	rBV	1241767	1959893	48.10%	7.410%
5	7.312	711	719	731	rBV	1265239	2268319	55.67%	8.576%
6	7.699	775	785	794	rBV	1223336	2064215	50.66%	7.804%
7	8.175	859	866	877	rVB	204040	349694	8.58%	1.322%
8	8.498	913	921	930	rVB	849699	1465386	35.96%	5.540%
9	9.350	1057	1066	1075	rBV	735391	1335288	32.77%	5.048%
10	10.995	1339	1346	1356	rVB	277622	509568	12.51%	1.927%
11	13.421	1749	1759	1768	rBV	1808776	2841733	69.74%	10.744%
12	14.238	1892	1898	1904	rBV	122478	179189	4.40%	0.677%
13	14.796	1986	1993	2002	rVB2	464567	737229	18.09%	2.787%
14	16.282	2239	2246	2263	rBV	1650463	2433407	59.72%	9.200%
15	17.539	2454	2460	2470	rBV2	620231	935988	22.97%	3.539%
16	18.397	2601	2606	2624	rBV2	213511	370803	9.10%	1.402%
17	19.660	2816	2821	2832	rBV2	94122	160209	3.93%	0.606%
18	19.918	2862	2865	2869	rVB2	43779	45894	1.13%	0.174%
19	20.135	2895	2902	2912	rBV	3152806	4074828	100.00%	15.406%
20	20.412	2941	2949	2954	rBV	49198	71963	1.77%	0.272%
21	20.782	3007	3012	3021	rBV8	24575	55958	1.37%	0.212%
22	20.905	3029	3033	3037	rBV	96382	110940	2.72%	0.419%
23	21.428	3116	3122	3134	rBV	408866	584612	14.35%	2.210%
24	21.827	3184	3190	3198	rVB2	649251	1109048	27.22%	4.193%
25	21.992	3210	3218	3225	rBV	118465	172099	4.22%	0.651%
26	22.626	3320	3326	3333	rBV	110155	195809	4.81%	0.740%
27	23.349	3443	3449	3459	rBV2	111147	218045	5.35%	0.824%
28	24.195	3586	3593	3601	rBV3	101520	204668	5.02%	0.774%
29	25.205	3753	3765	3780	rBV4	419467	1299654	31.89%	4.914%
30	26.403	3958	3969	3980	rVB4	50646	159294	3.91%	0.602%
31	26.533	3984	3991	4005	rVV7	27206	94494	2.32%	0.357%
32	27.843	4208	4214	4225	rVB4	25636	78945	1.94%	0.298%

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Instrument :
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ClientSampleId :
A0C12-SS4-10.0-10.5

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-BG012919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

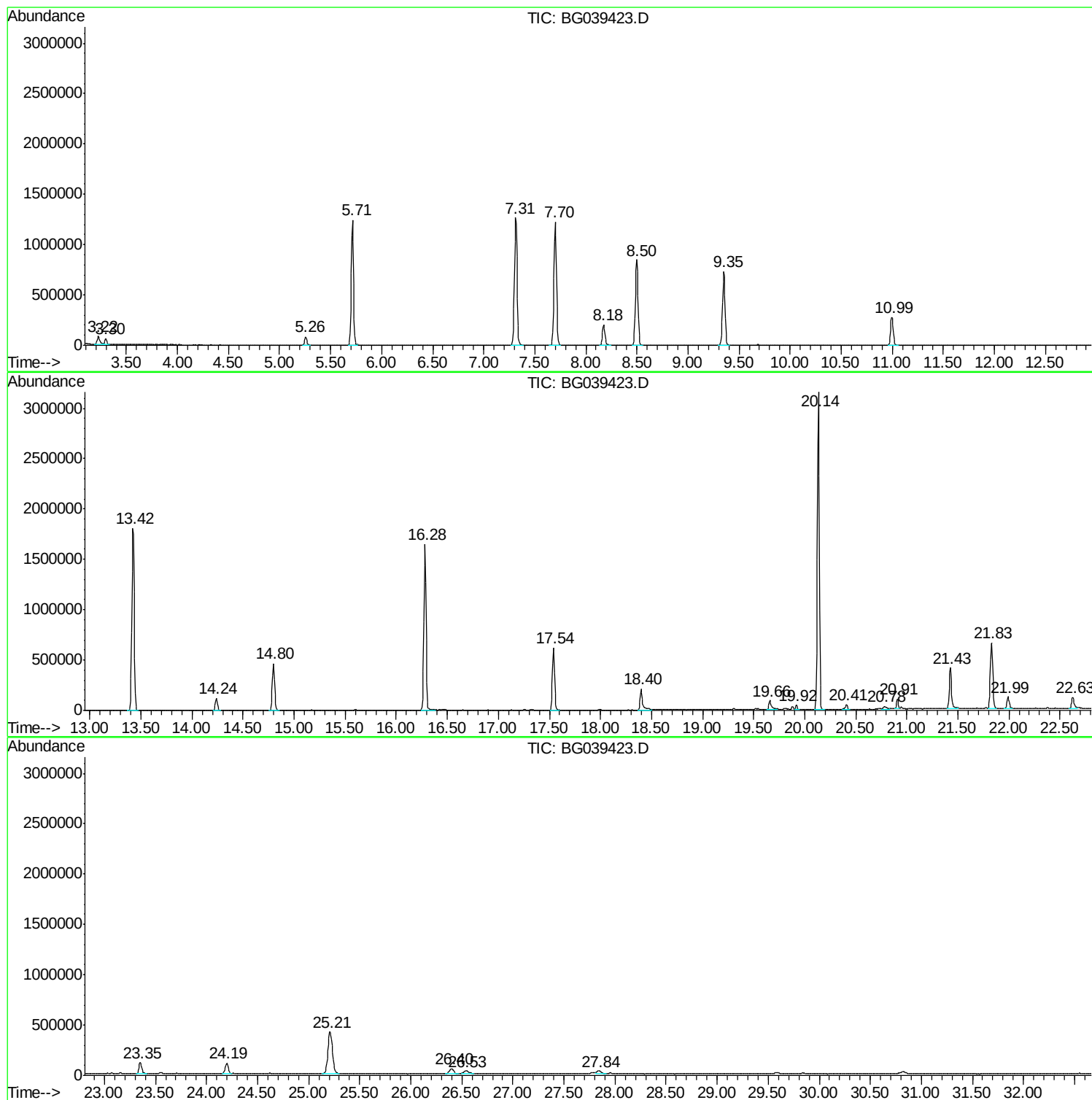
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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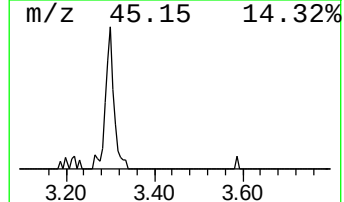
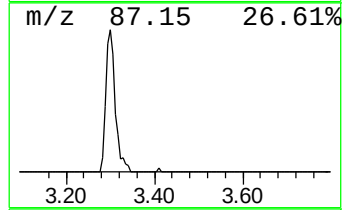
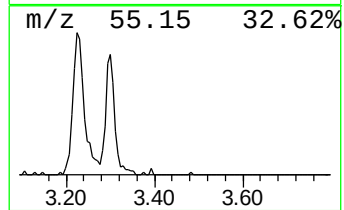
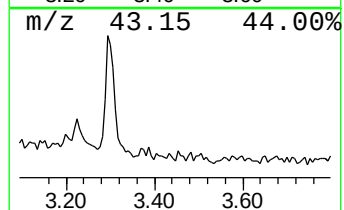
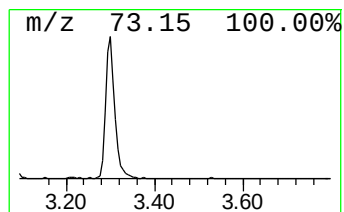
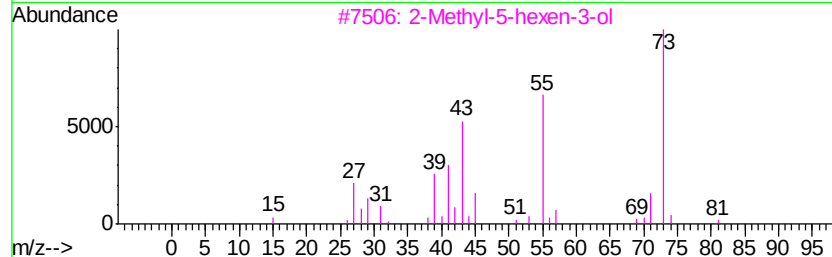
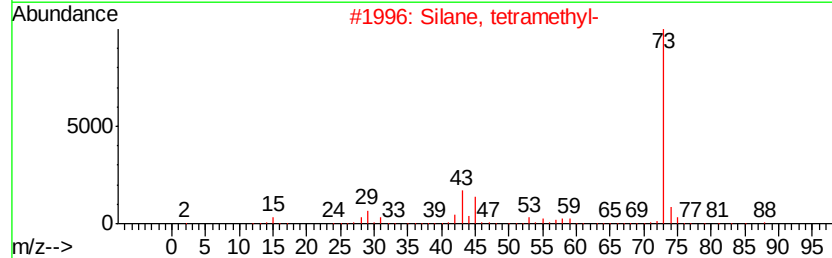
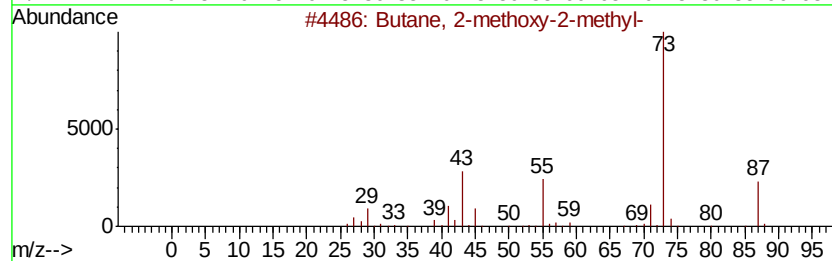
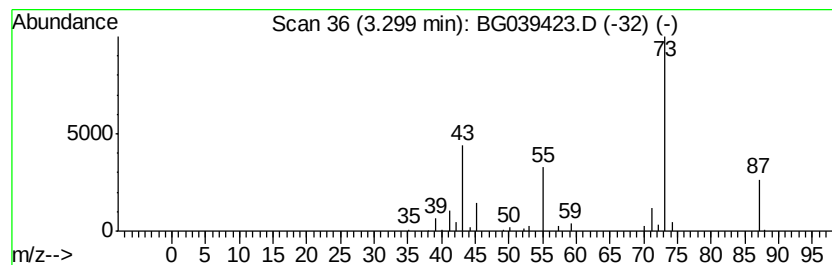
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.30	4.81 ng	84017	1,4-Dichlorobenzene-d4	8.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	1-(2-Methoxvethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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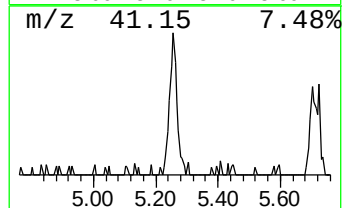
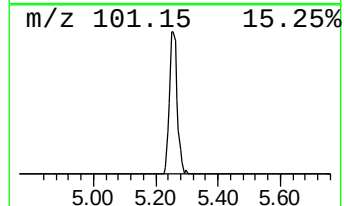
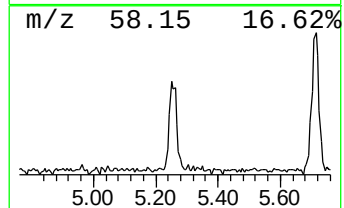
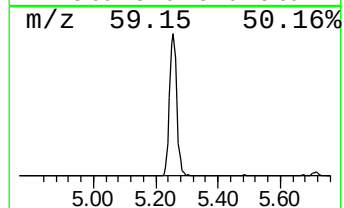
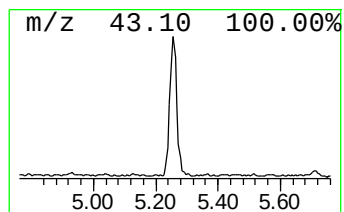
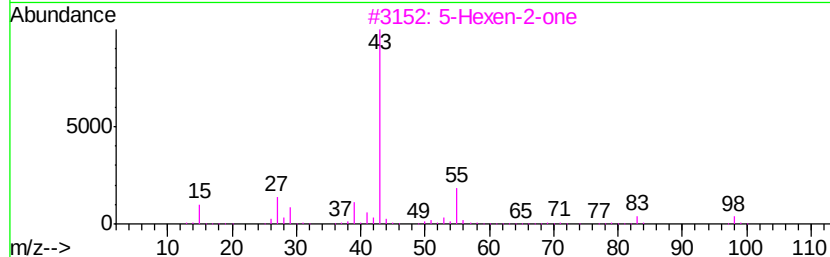
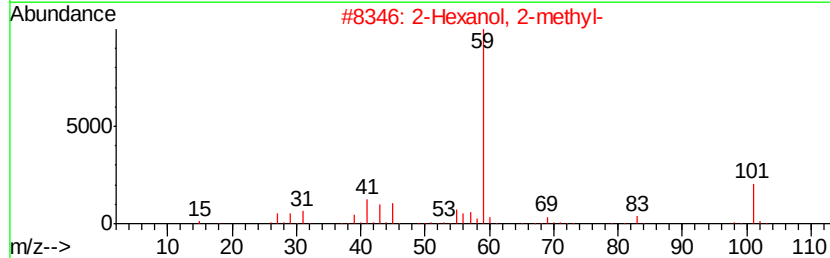
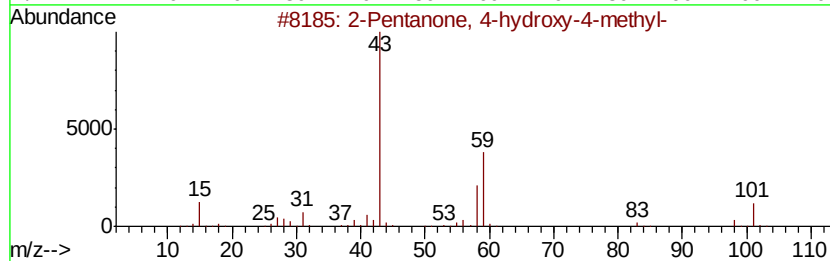
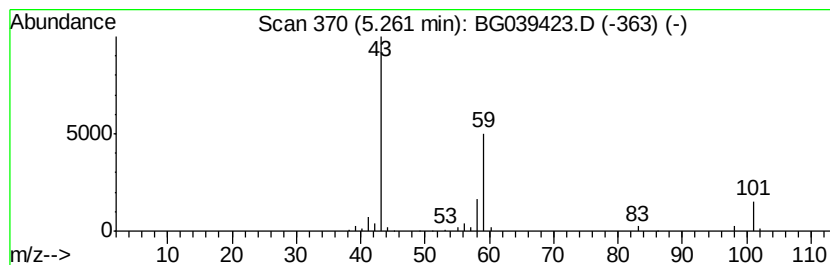
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	7.32 ng	128006	1,4-Dichlorobenzene-d4	8.18

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5			Propane-1,1-diol diacetate	160	C7H12O4	033931-80-5	9



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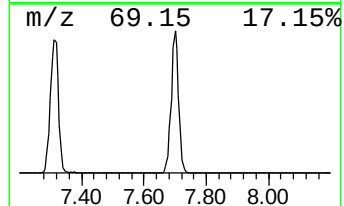
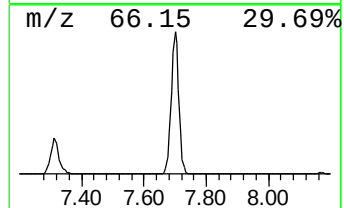
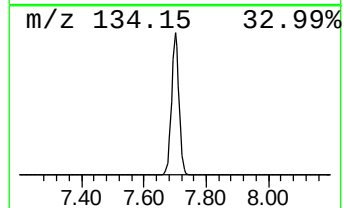
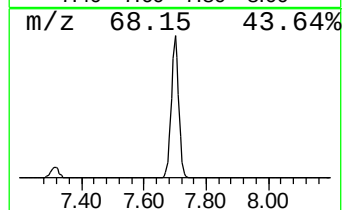
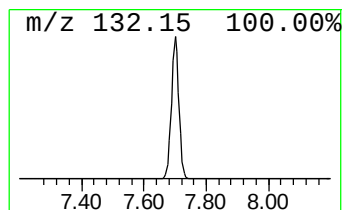
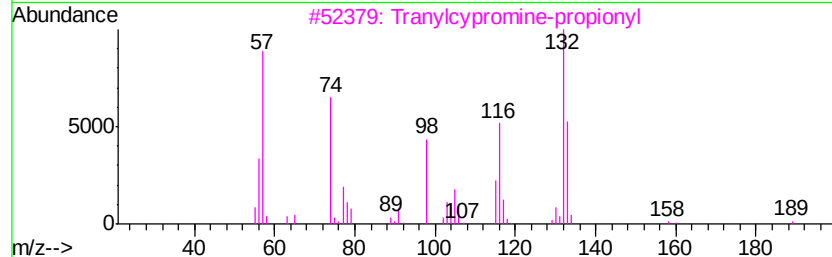
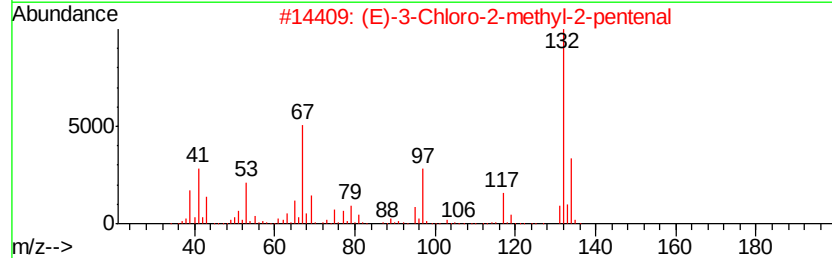
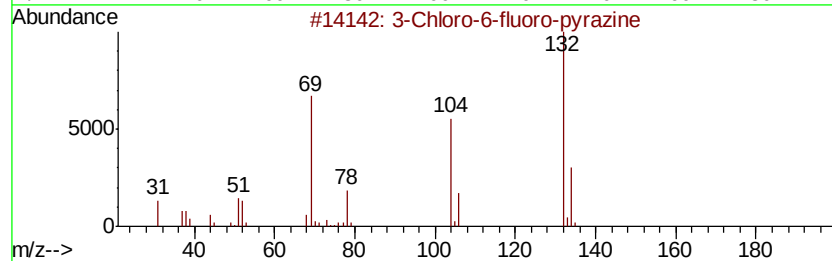
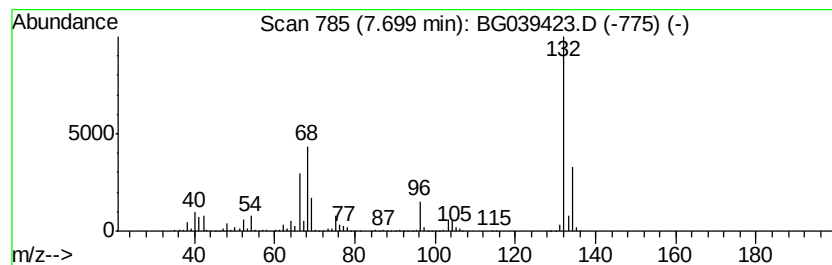
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Peak Number 4 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	118.06 ng	2064220	1,4-Dichlorobenzene-d4	8.18

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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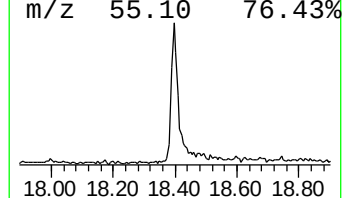
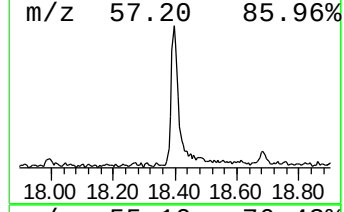
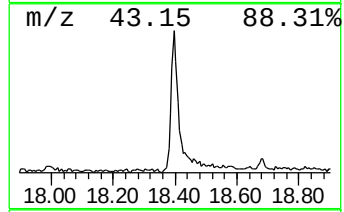
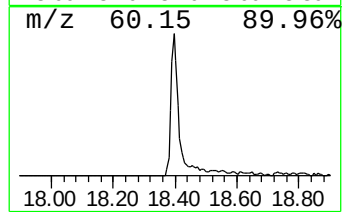
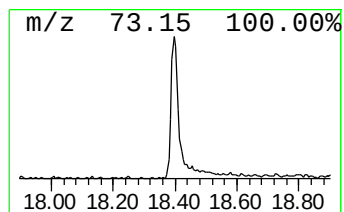
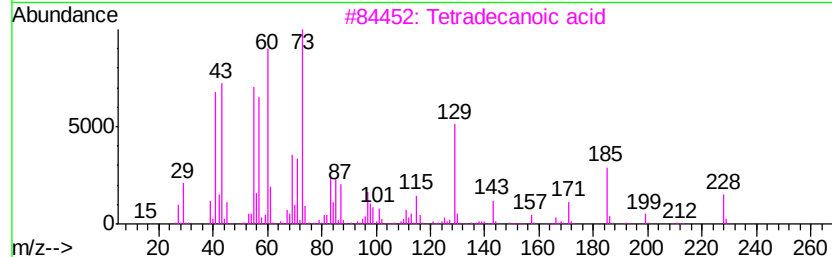
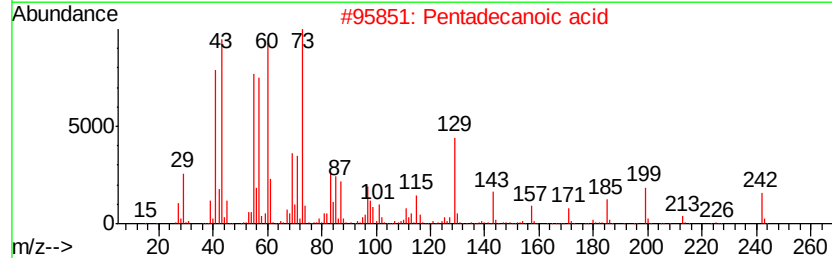
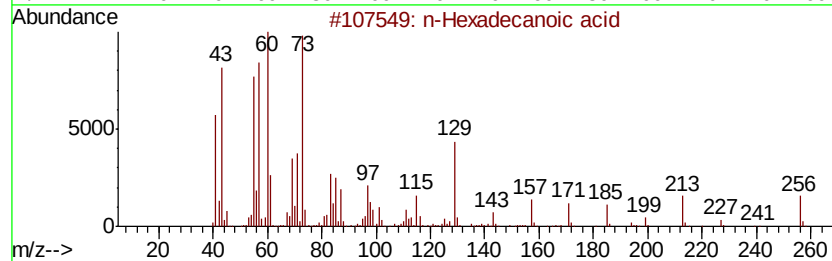
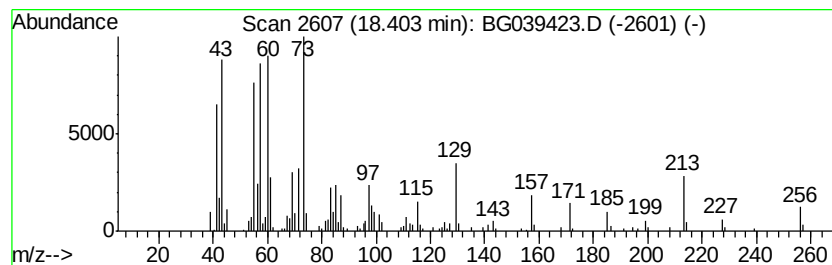
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.40	7.92 ng	370803	Phenanthrene-d10	17.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	11



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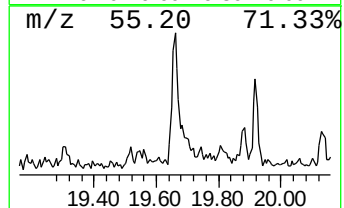
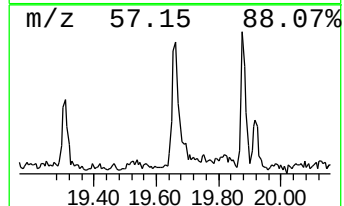
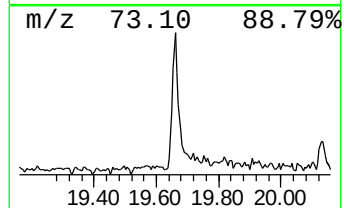
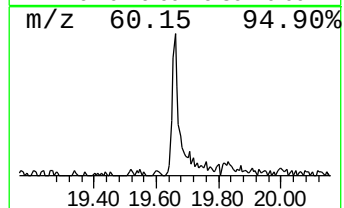
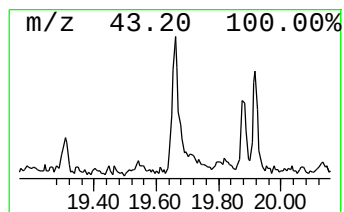
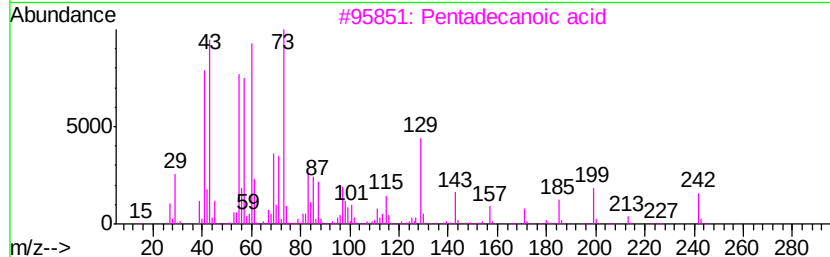
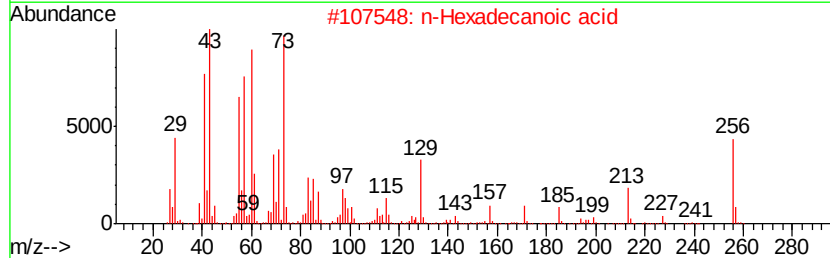
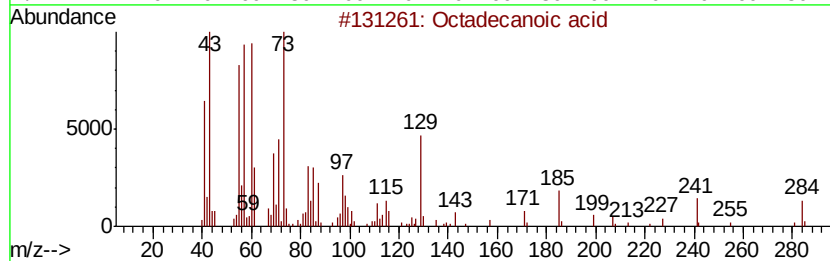
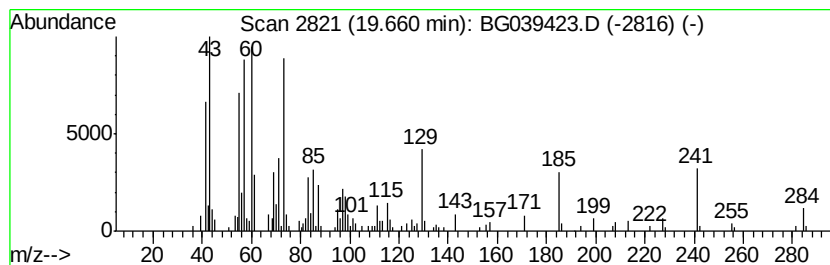
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Peak Number 7 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.66	3.42 ng	160209	Phenanthrene-d10		17.54
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	59



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ClientSampleId :
A0C12-SS4-10.0-10.5

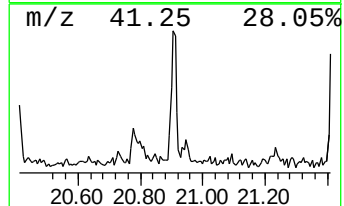
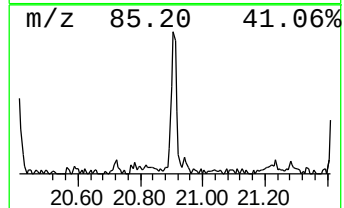
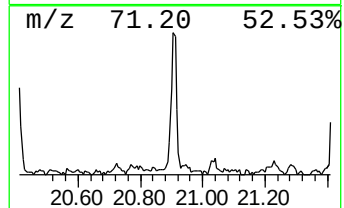
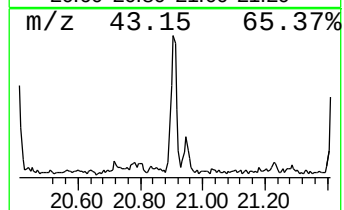
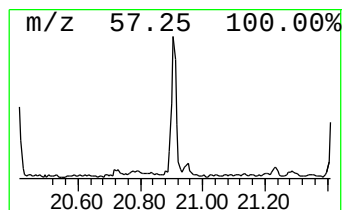
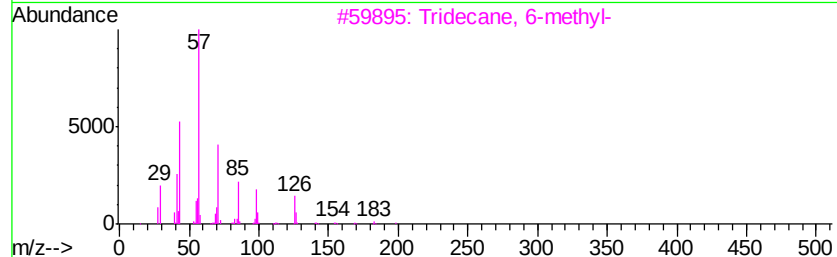
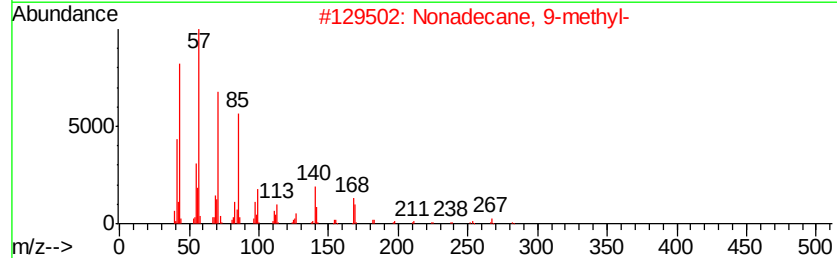
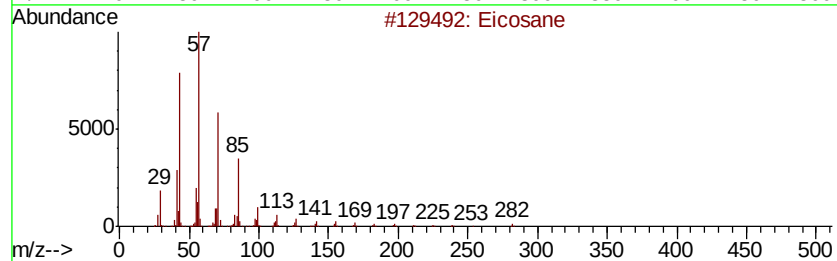
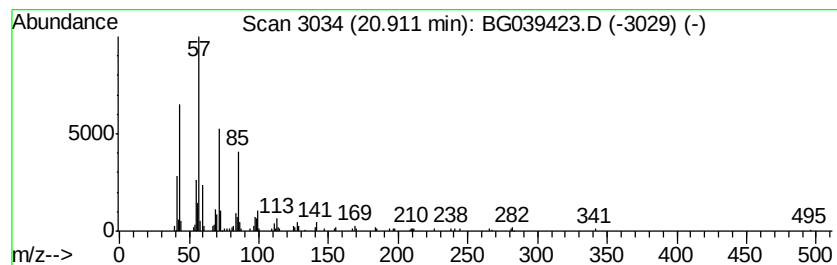
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.91	2.00 ng	110940	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	98
2		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86
3		Tridecane, 6-methyl-	198	C14H30	013287-21-3	62
4		Pentadecane	212	C15H32	000629-62-9	62
5		Tetracosane	338	C24H50	000646-31-1	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020819\
Data File : BG039423.D
Acq On : 8 Feb 2019 19:54
Operator : JU/SJ
Sample : K1404-08
Misc :
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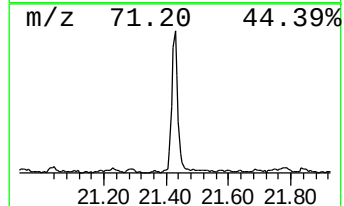
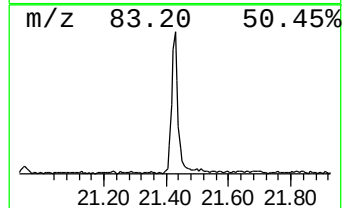
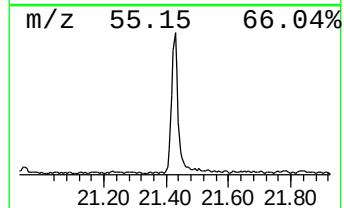
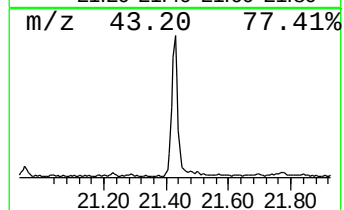
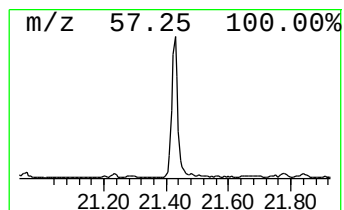
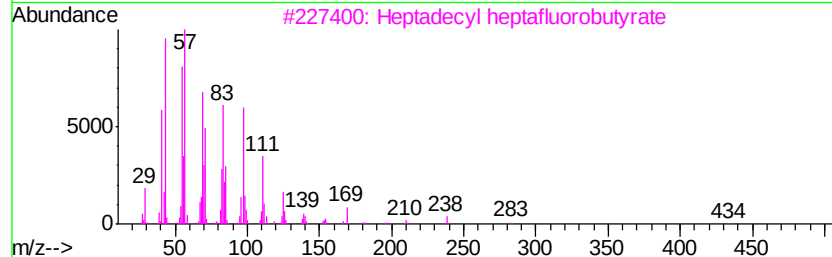
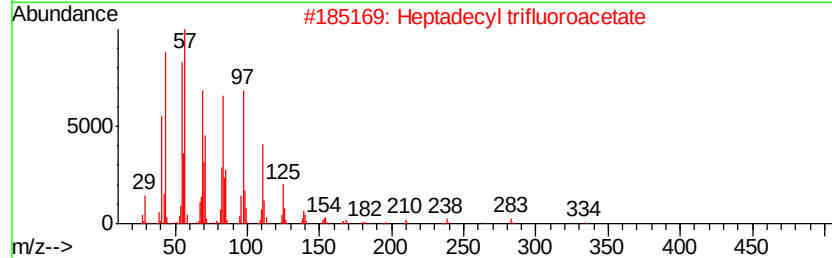
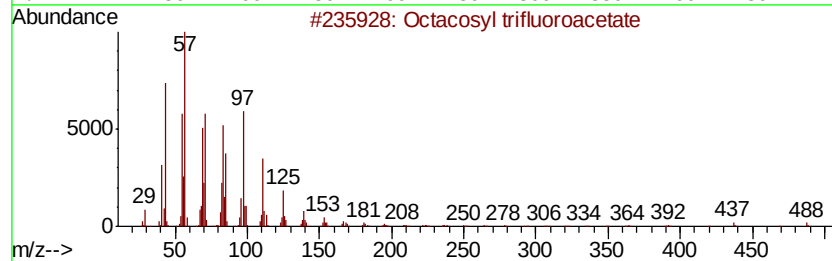
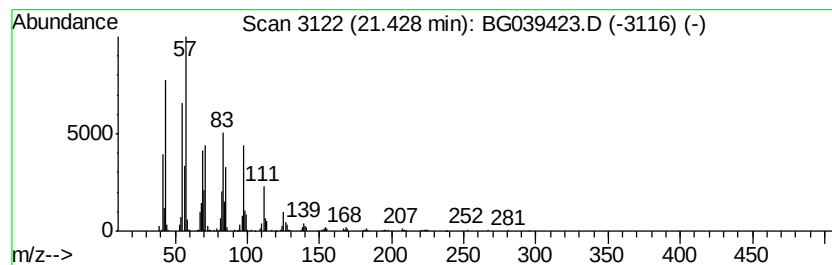
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.43	10.54 ng	584612	Chrysene-d12	21.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020819\
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Sample : K1404-08
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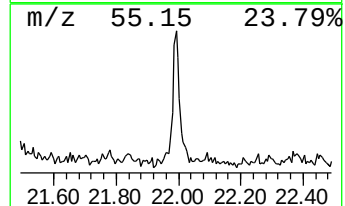
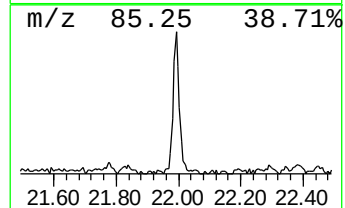
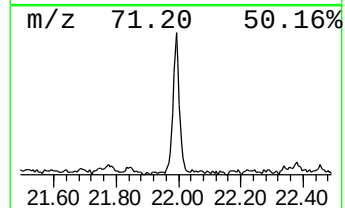
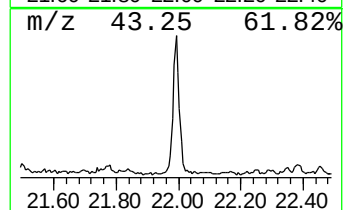
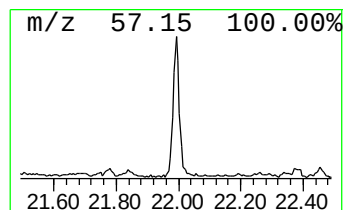
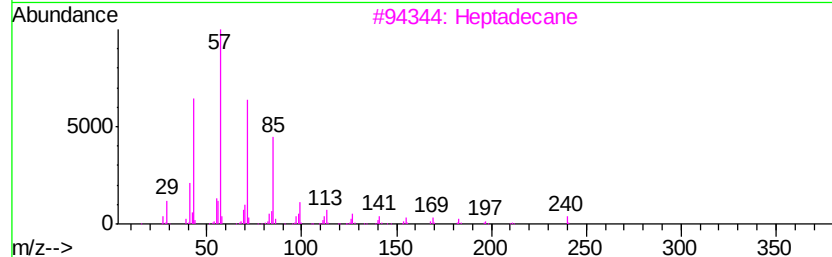
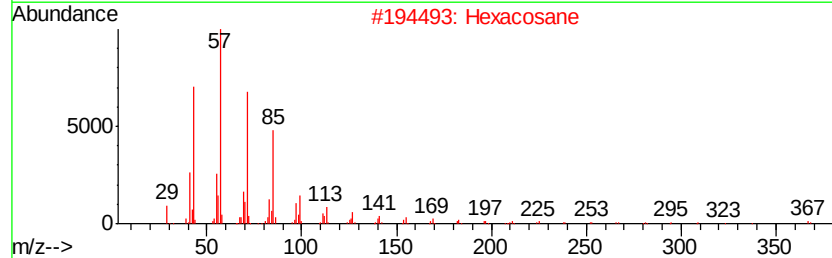
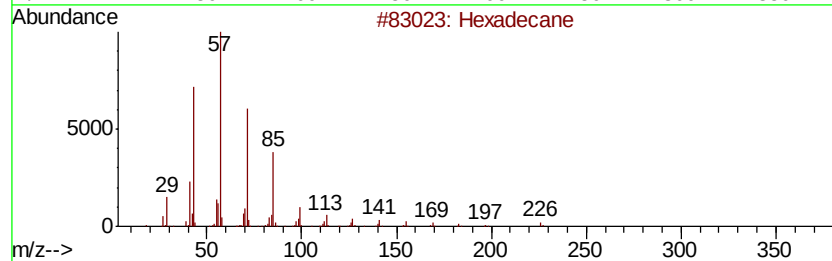
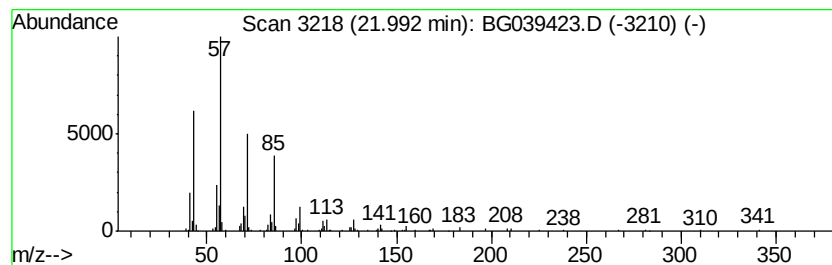
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.99	3.10 ng	172099	Chrysene-d12		21.83	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	87
2	Hexacosane		366	C26H54	000630-01-3	87
3	Heptadecane		240	C17H36	000629-78-7	86
4	Heneicosane		296	C21H44	000629-94-7	83
5	Eicosane, 9-octyl-		394	C28H58	013475-77-9	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020819\
Data File : BG039423.D
Acq On : 8 Feb 2019 19:54
Operator : JU/SJ
Sample : K1404-08
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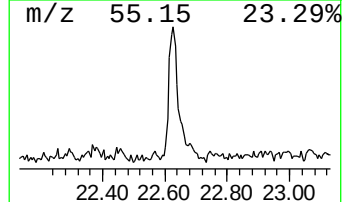
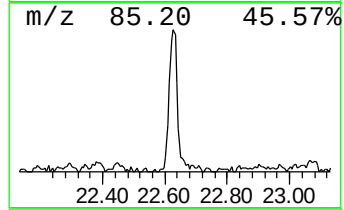
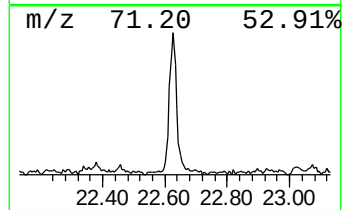
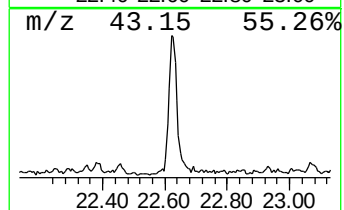
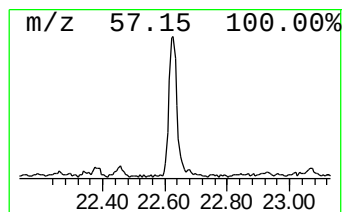
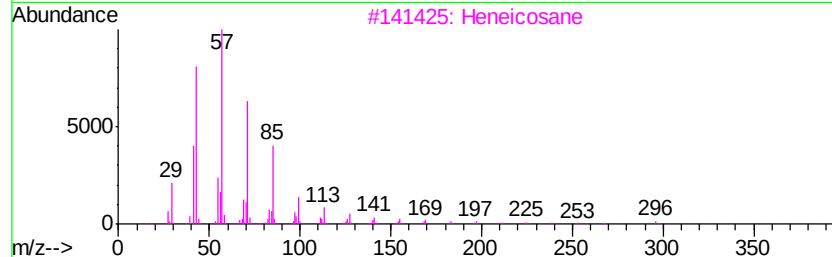
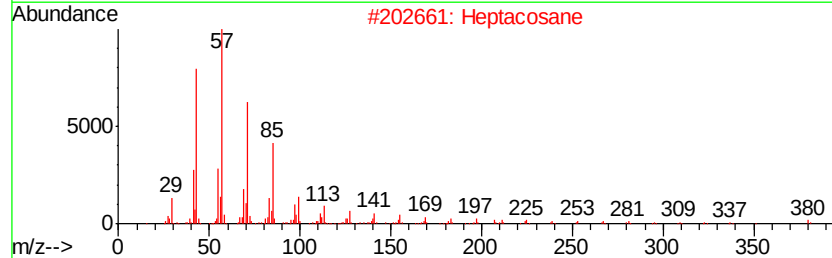
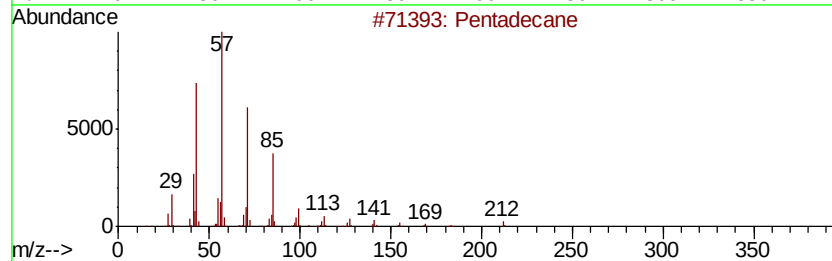
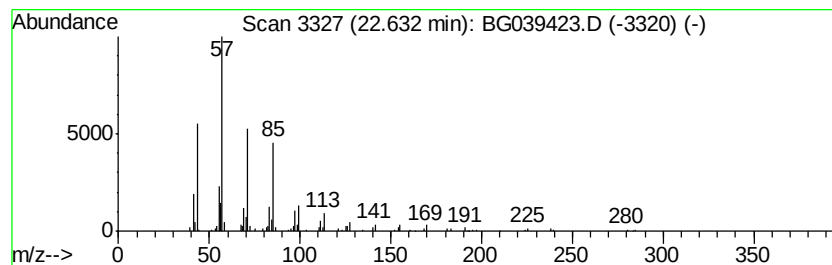
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	3.53 ng	195809	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	93
2		Heptacosane	380	C27H56	000593-49-7	90
3		Heneicosane	296	C21H44	000629-94-7	87
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020819\
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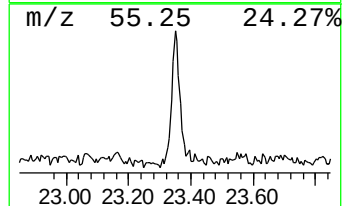
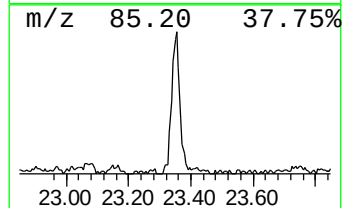
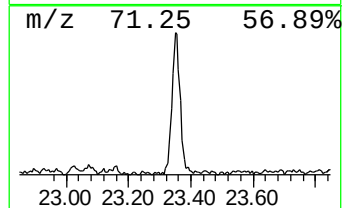
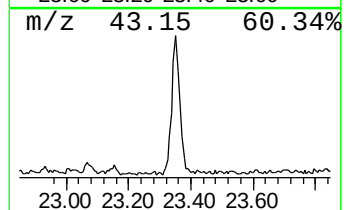
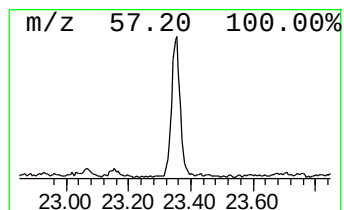
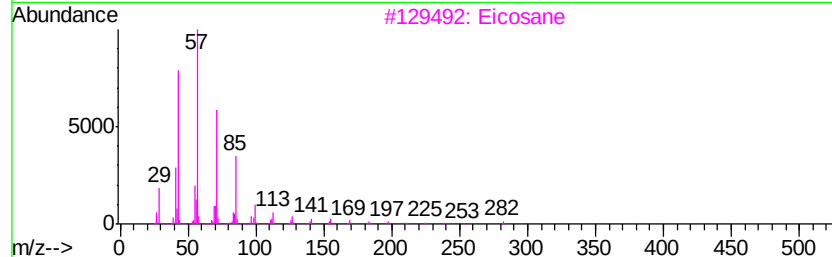
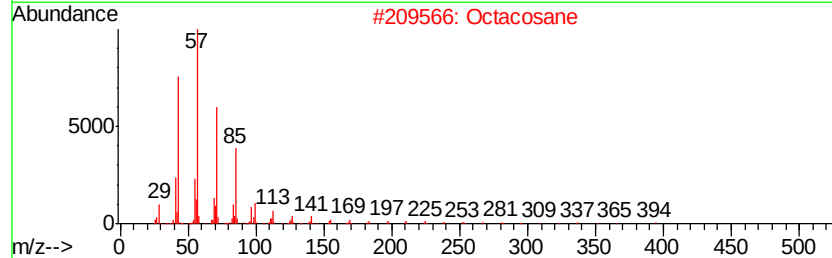
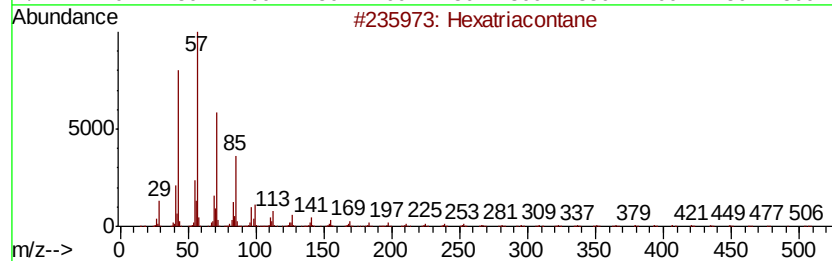
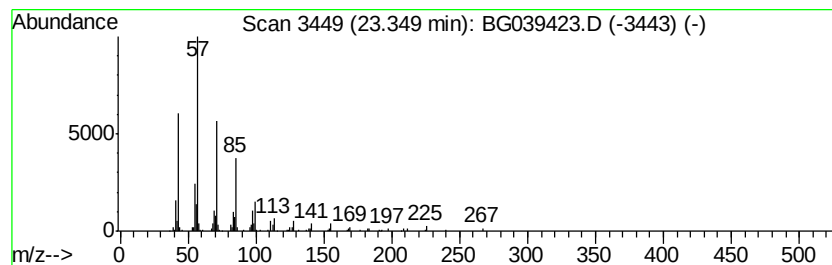
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	3.93 ng	218045	Chrysene-d12	21.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexatriacontane	507	C36H74	000630-06-8	91
2		Octacosane	394	C28H58	000630-02-4	90
3		Eicosane	282	C20H42	000112-95-8	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020819\
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Acq On : 8 Feb 2019 19:54
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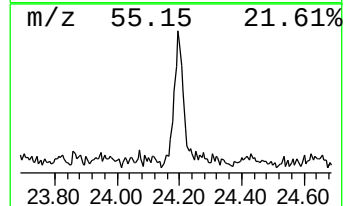
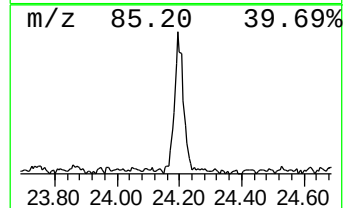
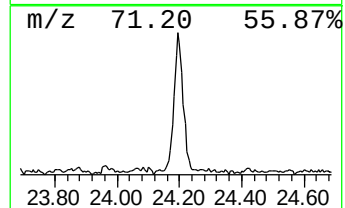
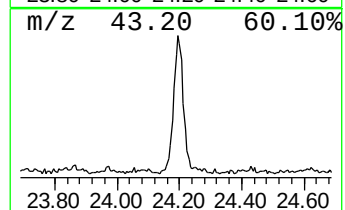
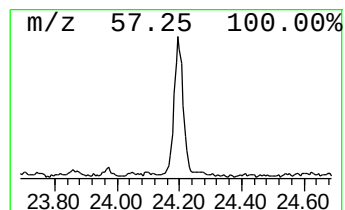
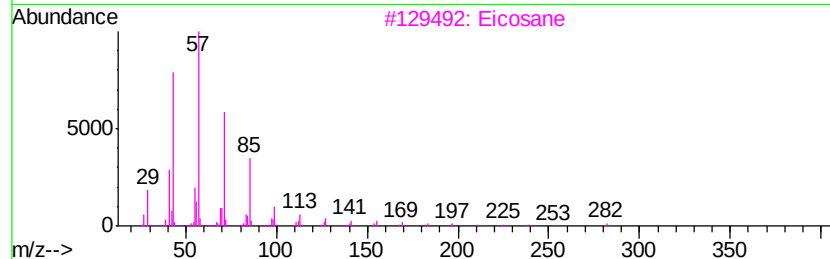
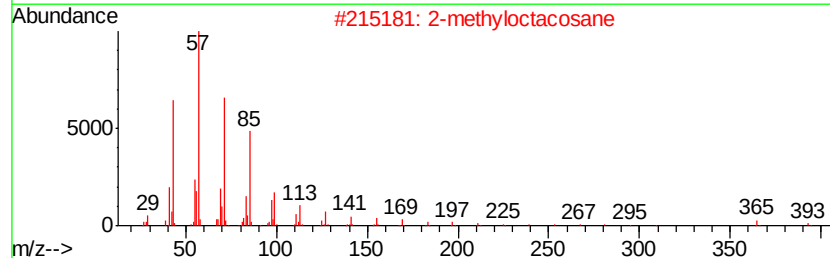
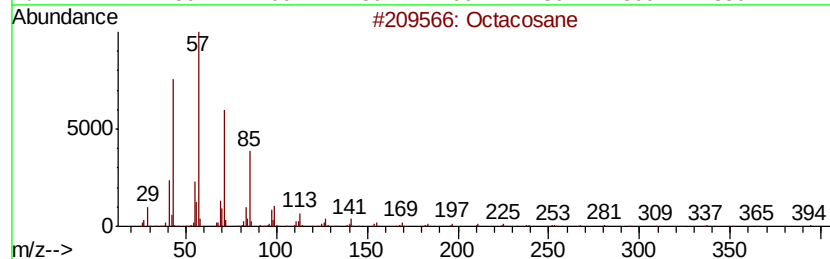
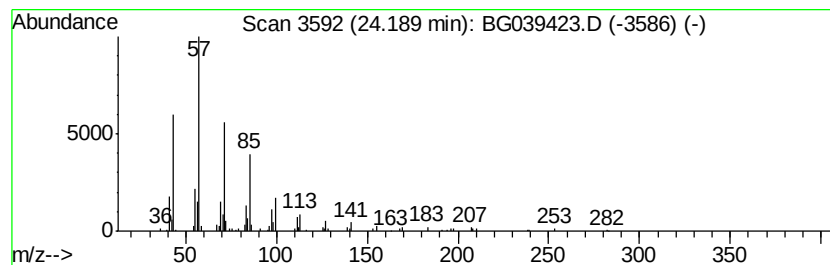
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.19	3.15 ng	204668	Perylene-d12	25.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	90
3			Eicosane	282	C20H42	000112-95-8	87
4			Octadecane	254	C18H38	000593-45-3	87
5			Hexadecane	226	C16H34	000544-76-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG020819\
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Misc :
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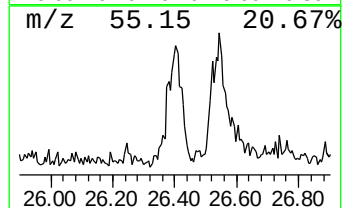
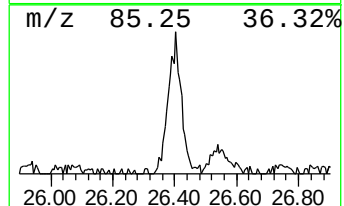
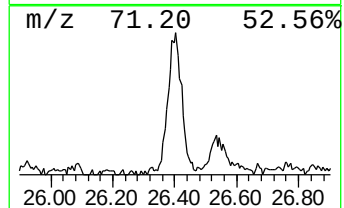
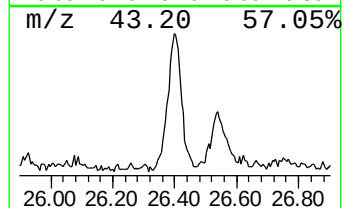
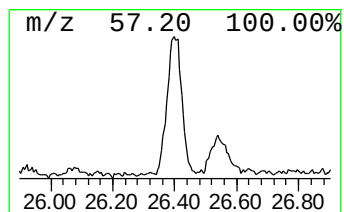
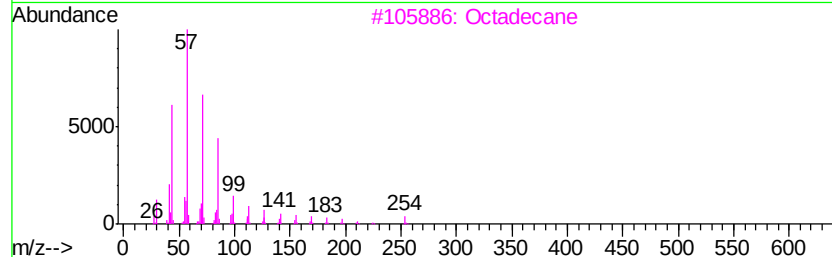
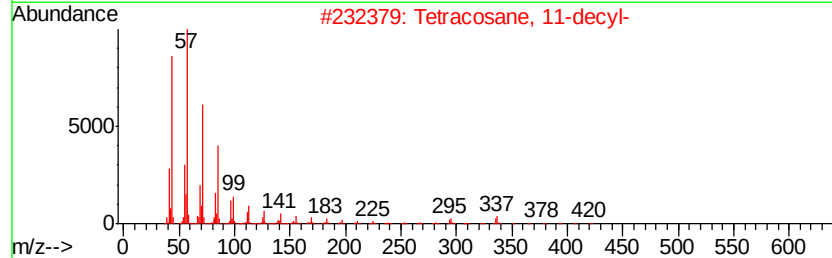
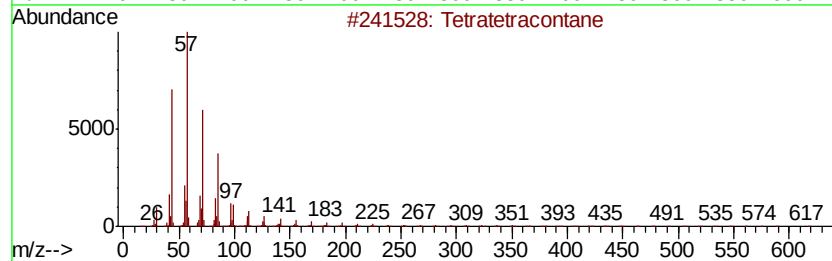
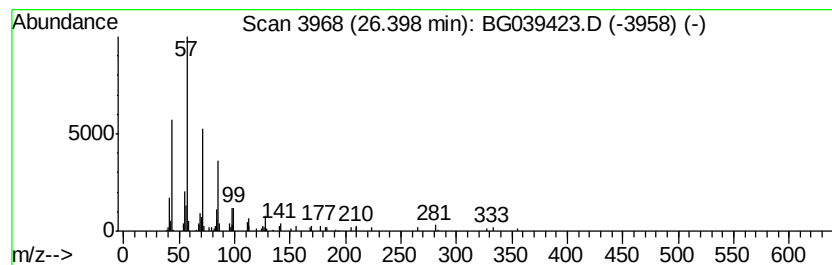
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Tetratetracontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.40	2.45 ng	159294	Perylene-d12	25.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	86
2		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86
3		Octadecane	254	C18H38	000593-45-3	80
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
5		Octacosane	394	C28H58	000630-02-4	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG020819\
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 Sample : K1404-08
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A0C12-SS4-10.0-10.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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...	3.30	4.8	ng	84017	1	8.18	349694	20.0
2-Pentanone, 4-hy...	5.26	7.3	ng	128006	1	8.18	349694	20.0
unknown7.70	7.70	118.1	ng	2064220	1	8.18	349694	20.0
n-Hexadecanoic acid	18.40	7.9	ng	370803	4	17.54	935988	20.0
Octadecanoic acid	19.66	3.4	ng	160209	4	17.54	935988	20.0
Eicosane	20.91	2.0	ng	110940	5	21.83	1109050	20.0
Octacosyl trifluo...	21.43	10.5	ng	584612	5	21.83	1109050	20.0
Hexadecane	21.99	3.1	ng	172099	5	21.83	1109050	20.0
Pentadecane	22.63	3.5	ng	195809	5	21.83	1109050	20.0
Hexatriacontane	23.35	3.9	ng	218045	5	21.83	1109050	20.0
Octacosane	24.19	3.1	ng	204668	6	25.21	1299650	20.0
Tetratetracontane	26.40	2.5	ng	159294	6	25.21	1299650	20.0