LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090119\
Data File : BG042675.D
Acq On : 1 Sep 2019 23:45
Operator : HP/JU
Sample : K4554-24
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11-(13-15)

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-BG082219.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	3.117	3	5	15	rVB	127133	156145	6.54%	1.429%
2	5.556	413	420	433	rBV	340977	559762	23.43%	5.122%
3	7.160	686	693	702	rBV	346011	620292	25.97%	5.675%
4	7.530	748	756	765	rBV	380551	664328	27.81%	6.078%
5	7.994	829	835	848	rVB	86405	143827	6.02%	1.316%
6	8.323	883	891	899	rBV	306554	536642	22.47%	4.910%
7	9.163	1027	1034	1052	rBV	201727	383260	16.04%	3.507%
8	10.820	1307	1316	1330	rBV	94816	196826	8.24%	1.801%
9	13.276	1726	1734	1749	rBV	752151	1237332	51.80%	11.321%
10	13.546	1774	1780	1791	rVB2	15583	26755	1.12%	0.245%
11	14.105	1868	1875	1890	rBV	47980	88780	3.72%	0.812%
12	14.657	1962	1969	1979	rBV	196812	328120	13.74%	3.002%
13	16.149	2216	2223	2238	rBV	628931	1070613	44.82%	9.796%
14	17.407	2430	2437	2451	rBV	289593	466587	19.53%	4.269%
15	19.146	2728	2733	2742	rBV	118205	183968	7.70%	1.683%
16	19.463	2783	2787	2791	rBV	25275	28694	1.20%	0.263%
17	20.021	2875	2882	2892	rBV	1772492	2388710	100.00%	21.856%
18	20.321	2930	2933	2939	rVB2	22076	31323	1.31%	0.287%
19	20.697	2991	2997	3005	rVB3	17509	29223	1.22%	0.267%
20	20.814	3012	3017	3022	rBV2	23620	29235	1.22%	0.267%
21	21.320	3099	3103	3114	rVV2	67331	133254	5.58%	1.219%
22	21.678	3158	3164	3177	rBV2	348996	607778	25.44%	5.561%
23	21.872	3193	3197	3201	rVB2	22020	31512	1.32%	0.288%
24	22.483	3296	3301	3305	rBV	32345	46593	1.95%	0.426%
25	23.176	3412	3419	3426	rBV	38709	72800	3.05%	0.666%
26	23.987	3550	3557	3565	rBV3	38905	82432	3.45%	0.754%
27	24.921	3703	3716	3733	rBV	223351	728124	30.48%	6.662%
28	26.073	3903	3912	3921	rBV5	18148	56624	2.37%	0.518%

Sum of corrected areas: 10929539

LSC Report - Integrated Chromatogram

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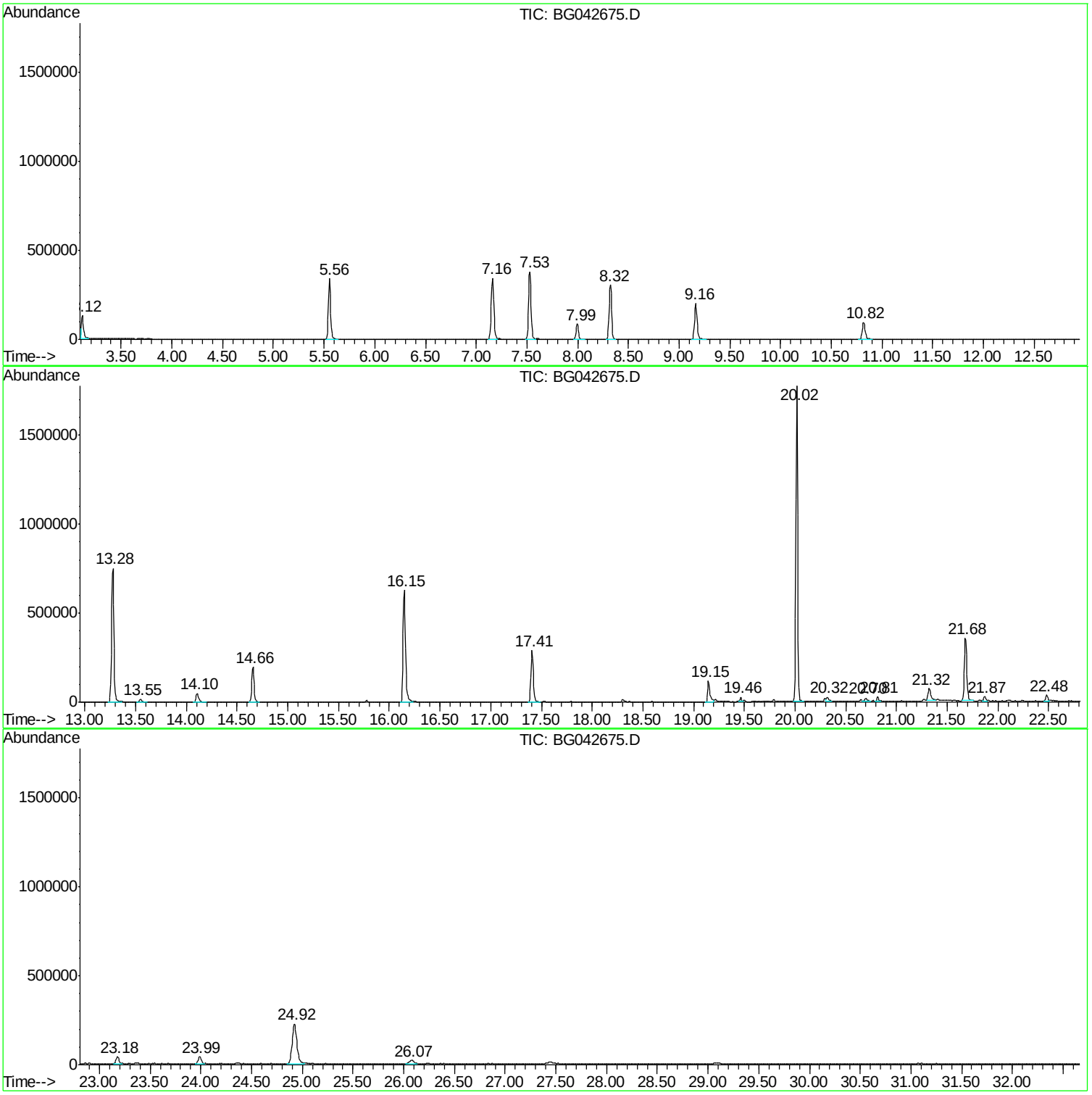
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11-(13-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : SB-11-(13-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

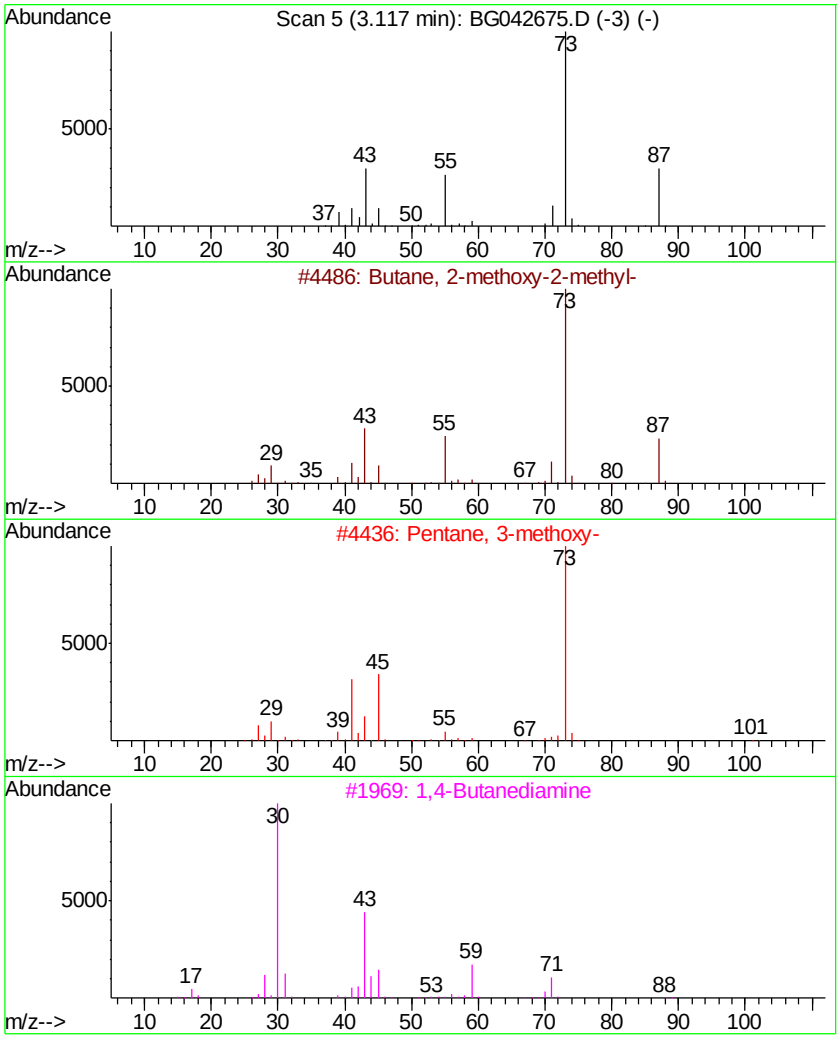
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

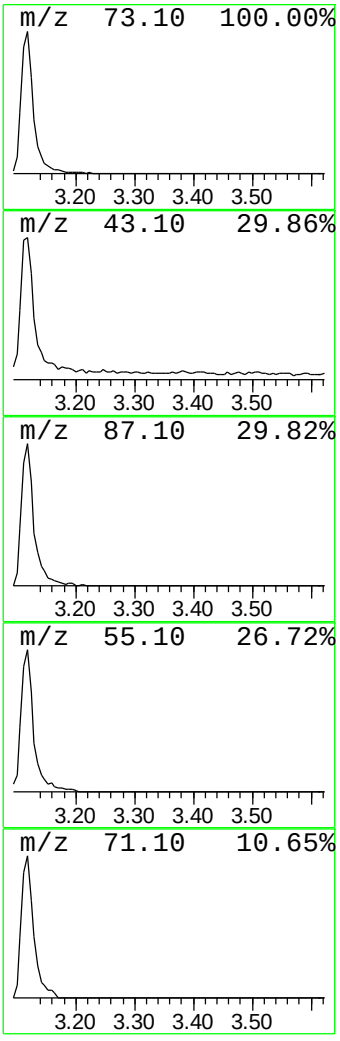
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	21.71 ng	156145	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	10
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





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Sample : K4554-24
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-11-(13-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.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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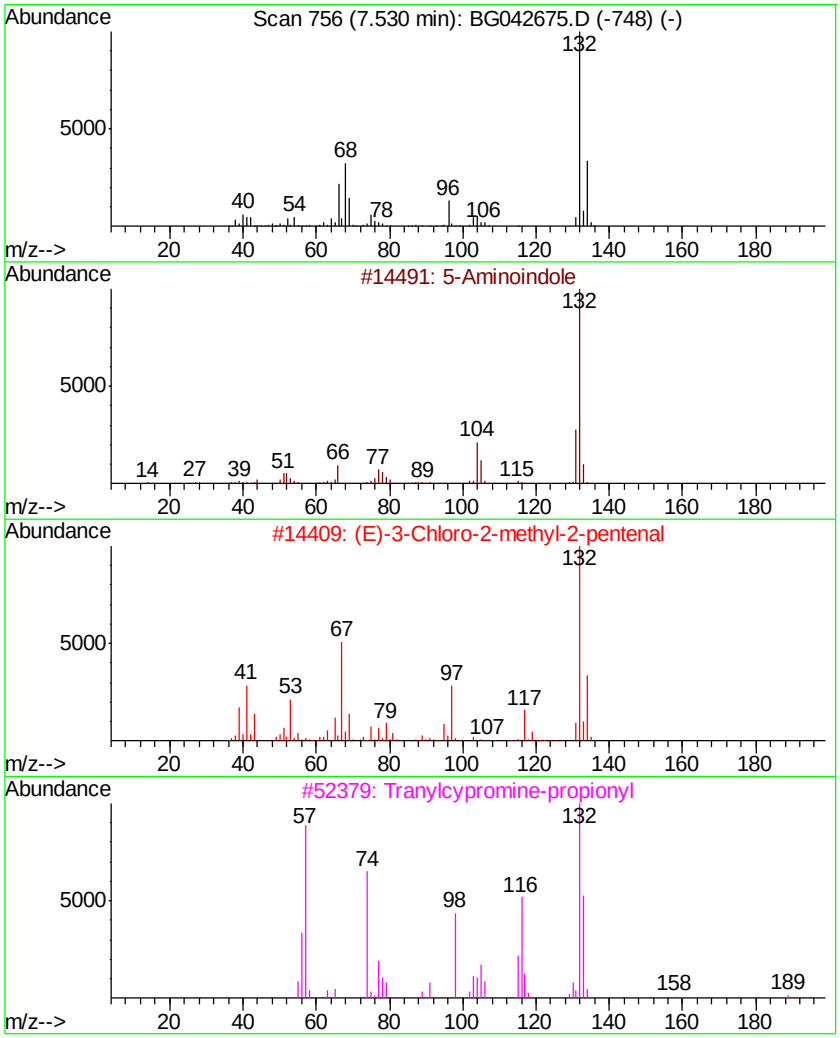
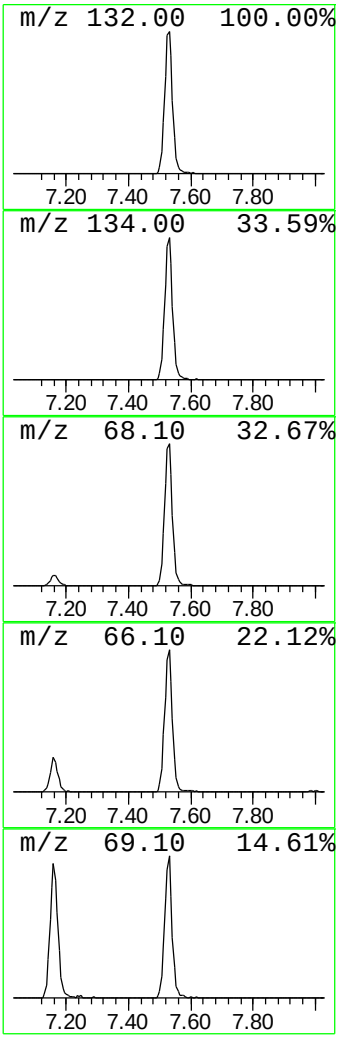
Peak Number 2 unknown7.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	92.38 ng	664328	1,4-Dichlorobenzene-d4	7.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	12
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : SB-11-(13-15)

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TIC Library : C:\Database\NIST11.L
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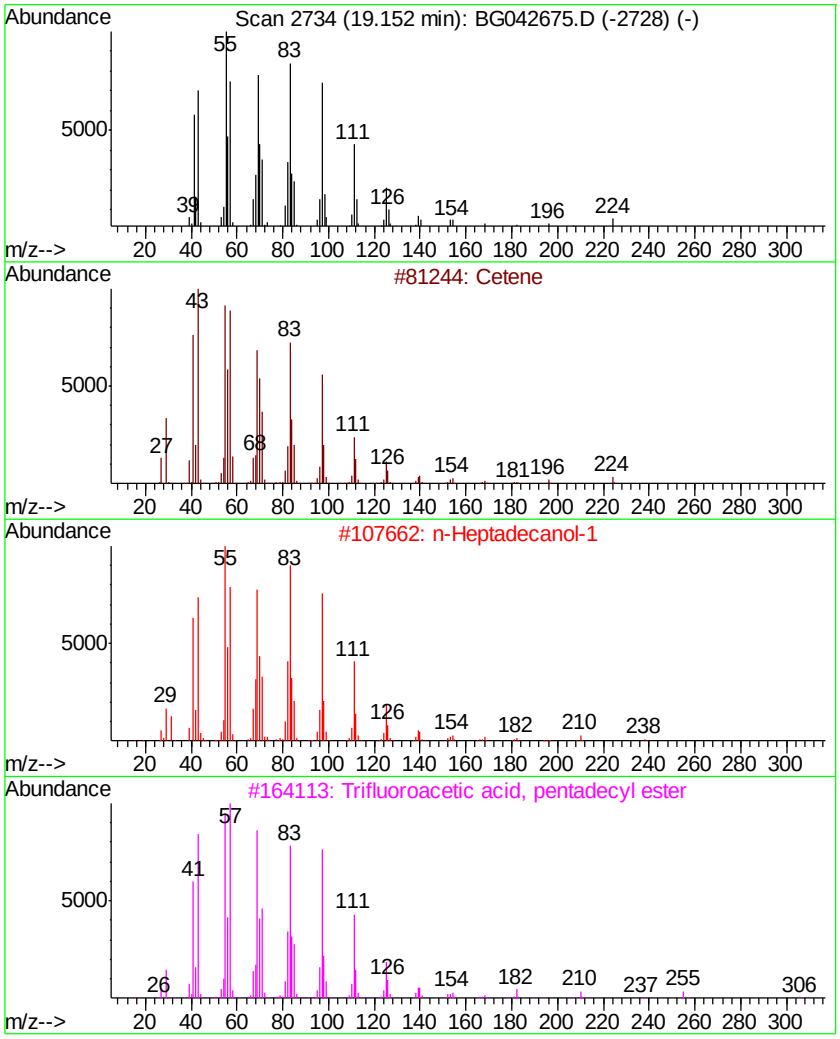
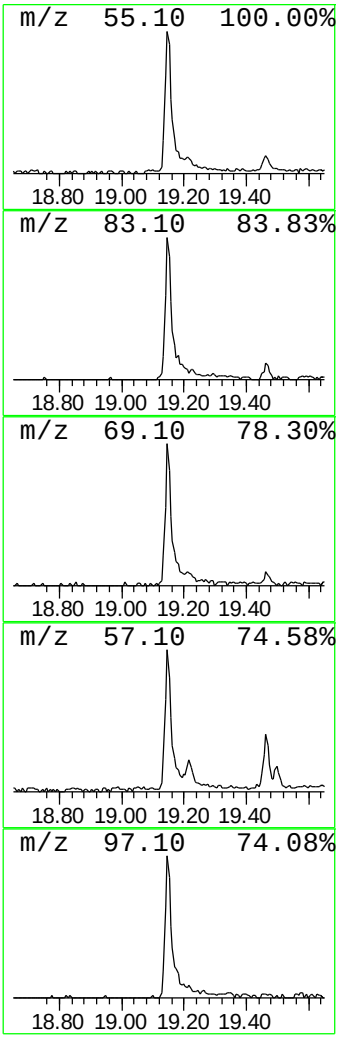
Peak Number 4 Cetene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.15	7.89 ng	183968	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





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Misc :
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Instrument : BNA_G
ClientSampleId : SB-11-(13-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
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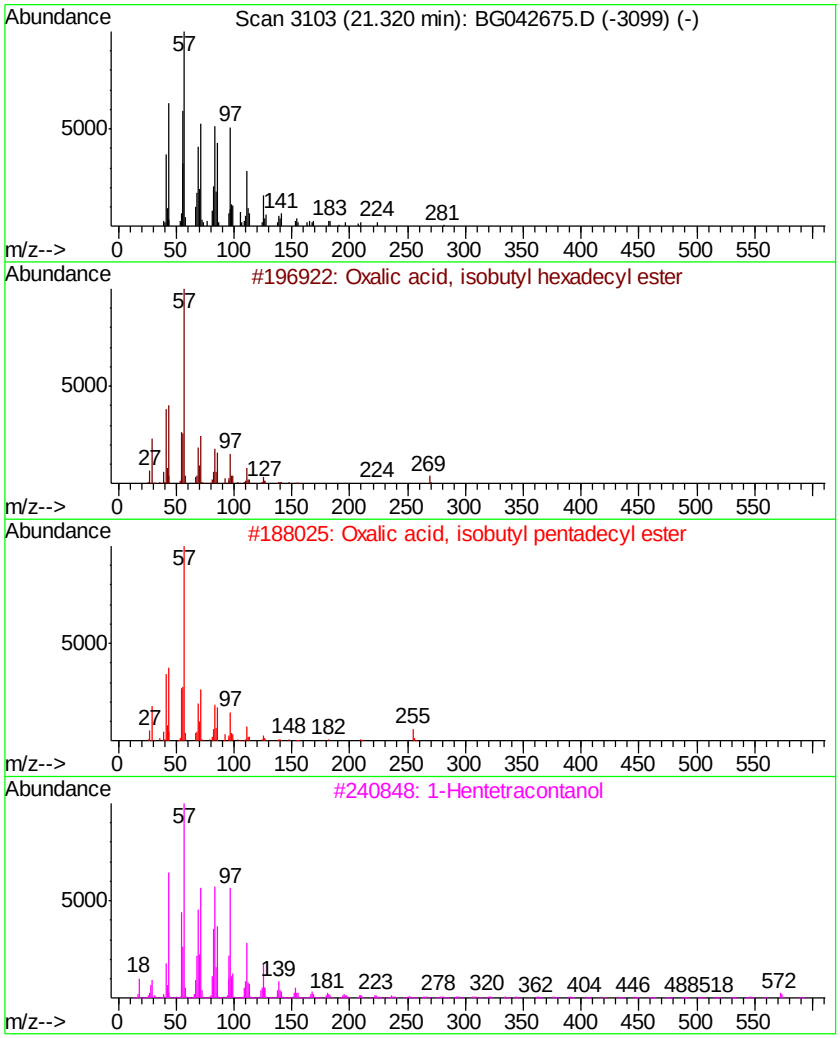
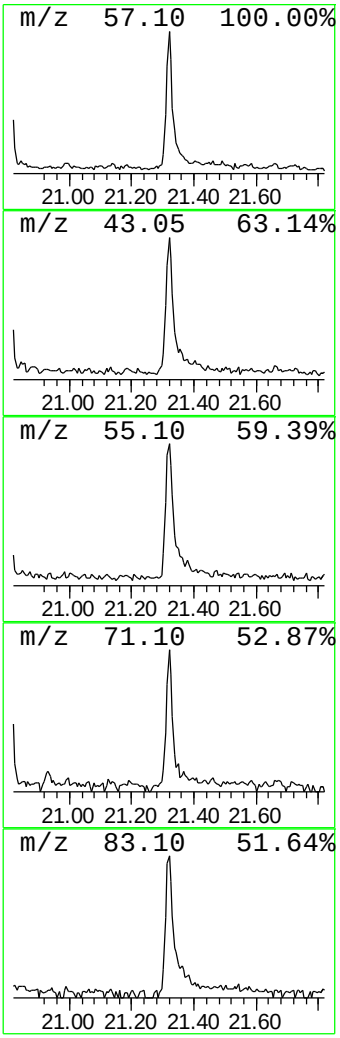
****

Peak Number 5 Oxalic acid, isobutyl hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	4.38 ng	133254	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
3	1-Hentetracontanol	593	C41H84O	040710-42-7	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
5	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : SB-11-(13-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082219.M
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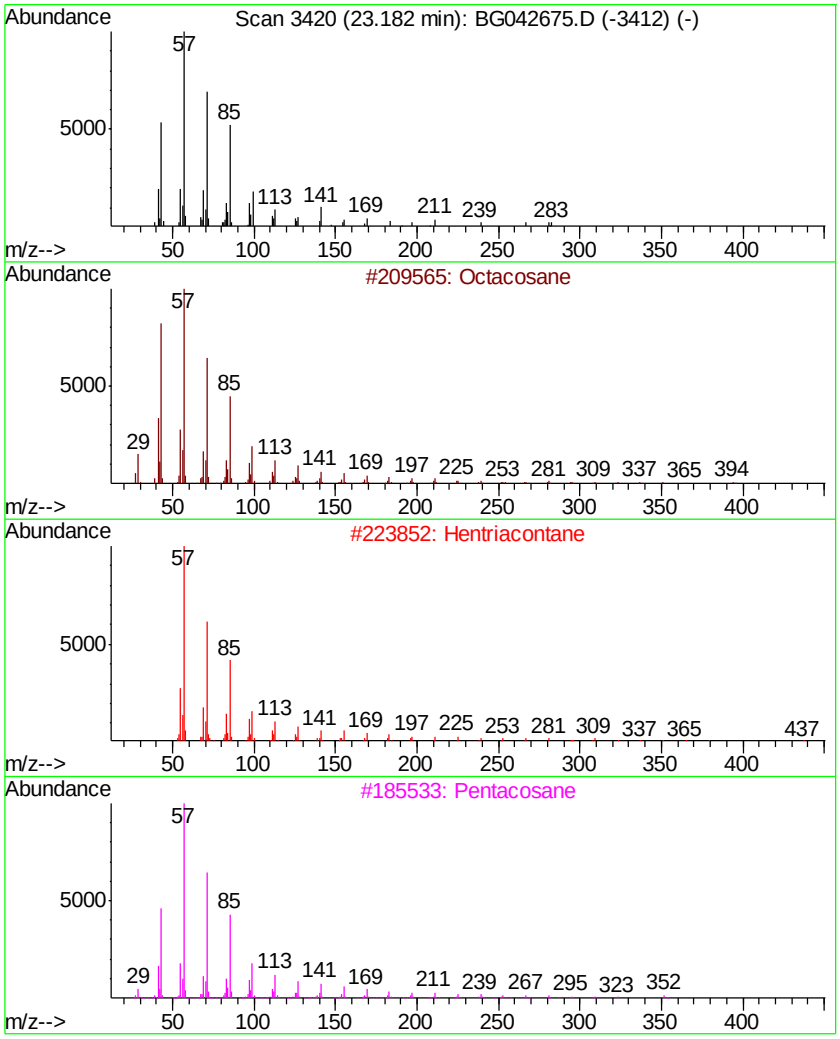
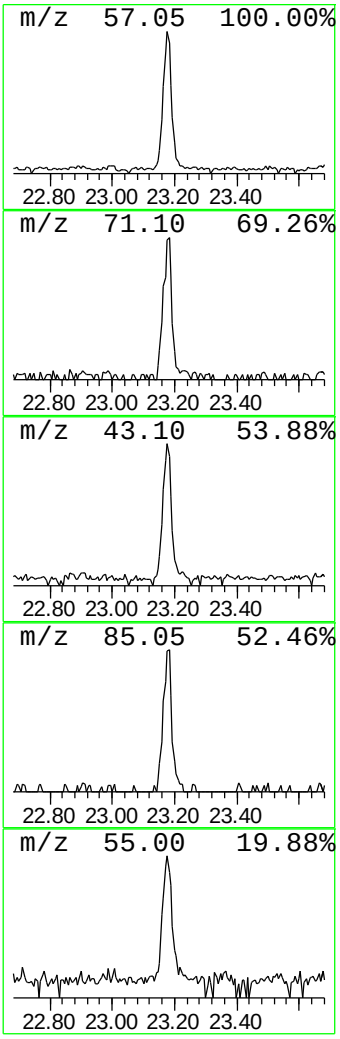
****

Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	2.40 ng	72800	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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TIC Library : C:\Database\NIST11.L
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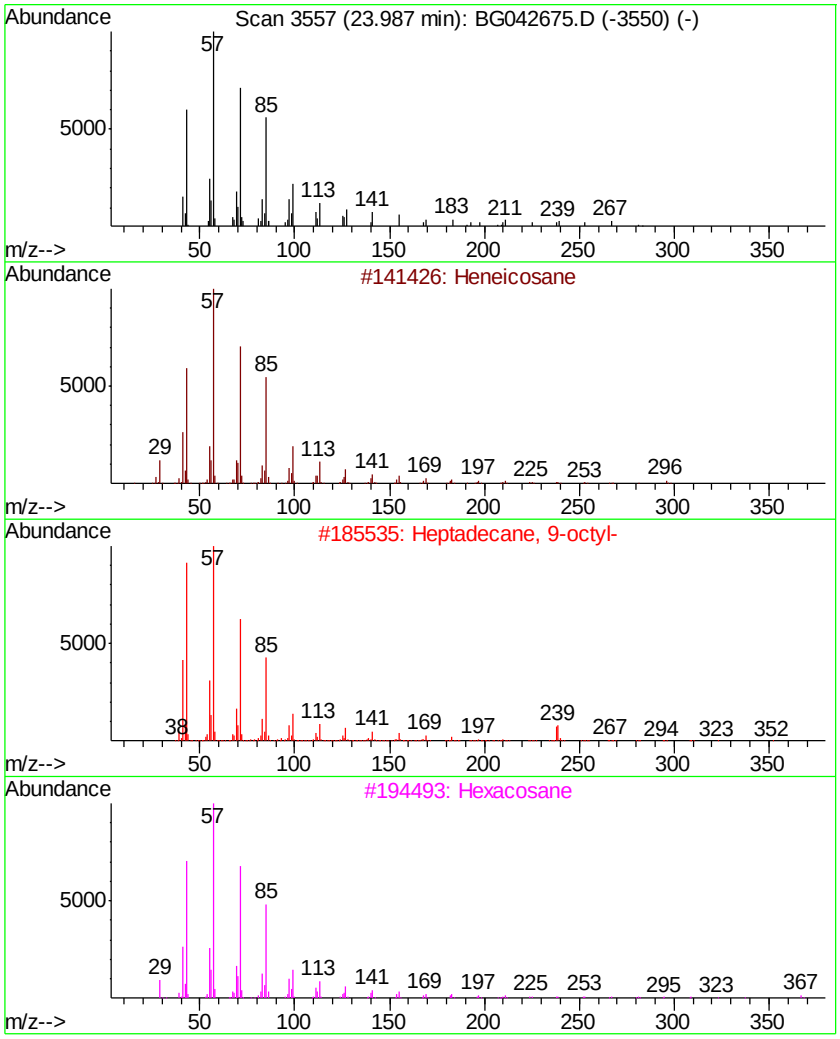
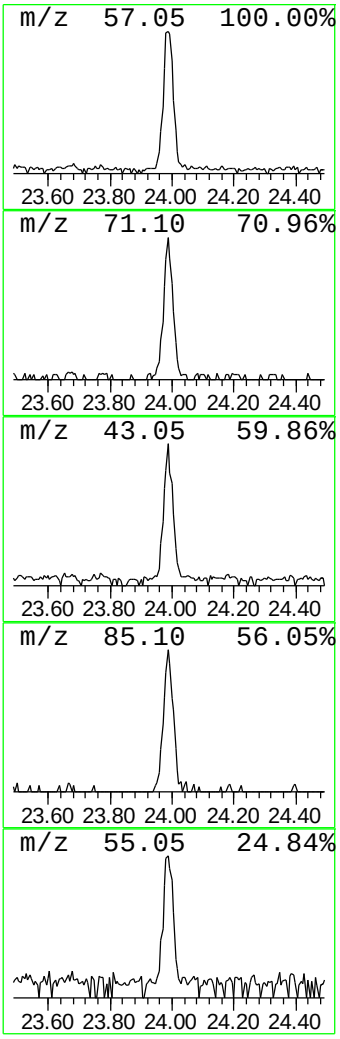
****

Peak Number 7 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	2.26 ng	82432	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.12	21.7	ng	156145	1	7.99	143827	20.0
unknown7.53	7.53	92.4	ng	664328	1	7.99	143827	20.0
Cetene	19.15	7.9	ng	183968	4	17.41	466587	20.0
Oxalic acid, isob...	21.32	4.4	ng	133254	5	21.68	607778	20.0
Octacosane	23.18	2.4	ng	72800	5	21.68	607778	20.0
Heneicosane	23.99	2.3	ng	82432	6	24.92	728124	20.0