LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042552.D
Acq On : 29 Aug 2019 3:57
Operator : HP/JU
Sample : K4543-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

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	22	rVB	118727	186567	9.56%	1.584%
2	5.555	413	420	431	rBV	293998	487868	25.00%	4.141%
3	7.159	686	693	710	rBV	286042	563733	28.89%	4.785%
4	7.529	748	756	769	rBV	322064	565498	28.98%	4.800%
5	8.000	829	836	846	rBV	100669	172010	8.81%	1.460%
6	8.323	882	891	906	rVB	263968	468851	24.02%	3.980%
7	9.163	1027	1034	1047	rBV	156260	314812	16.13%	2.672%
8	10.820	1306	1316	1328	rBV	109317	224676	11.51%	1.907%
9	13.276	1727	1734	1754	rBV	552749	920371	47.16%	7.812%
10	14.110	1869	1876	1886	rBV	37808	76209	3.90%	0.647%
11	14.656	1963	1969	1978	rBV	221048	361263	18.51%	3.066%
12	16.149	2217	2223	2240	rBV	466627	859470	44.04%	7.295%
13	17.412	2430	2438	2443	rBV	329447	535275	27.43%	4.544%
14	17.453	2443	2445	2453	rVB	41212	53180	2.72%	0.451%
15	18.293	2583	2588	2592	rBV	14583	22518	1.15%	0.191%
16	18.340	2592	2596	2606	rVB	18281	29038	1.49%	0.246%
17	18.481	2615	2620	2624	rBV2	17960	32729	1.68%	0.278%
18	18.834	2676	2680	2689	rVB4	10057	19939	1.02%	0.169%
19	19.204	2737	2743	2748	rBV3	20689	37414	1.92%	0.318%
20	19.345	2763	2767	2773	rBV3	11480	22068	1.13%	0.187%
21	19.463	2780	2787	2794	rBV	123914	182471	9.35%	1.549%
22	19.827	2840	2849	2857	rBV	138638	238790	12.24%	2.027%
23	19.903	2857	2862	2868	rVB4	13419	21396	1.10%	0.182%
24	20.021	2876	2882	2893	rVB	1463321	1951646	100.00%	16.566%
25	20.150	2898	2904	2905	rBV2	15844	24345	1.25%	0.207%
26	20.285	2922	2927	2928	rBV5	14798	19999	1.02%	0.170%
27	20.320	2929	2933	2937	rVB2	34108	54994	2.82%	0.467%
28	20.473	2954	2959	2963	rVV2	23584	35181	1.80%	0.299%
29	20.614	2979	2983	2987	rBV	19593	27137	1.39%	0.230%
30	20.661	2987	2991	2994	rVV	20257	29536	1.51%	0.251%
31	20.820	3015	3018	3022	rBV2	22618	25836	1.32%	0.219%
32	21.084	3059	3063	3067	rVB	18757	24723	1.27%	0.210%
33	21.266	3084	3094	3098	rBV3	22317	53357	2.73%	0.453%
34	21.325	3098	3104	3115	rVV4	74699	178100	9.13%	1.512%

LSC Area Percent Report

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Acq On : 29 Aug 2019 3:57
Operator : HP/JU
Sample : K4543-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

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

35	21.566	3143	3145	3150	rVB	14683	19594	1.00%	0.166%
36	21.683	3156	3165	3171	rBV3	495764	966240	49.51%	8.202%
37	21.730	3171	3173	3184	rVB	80583	121827	6.24%	1.034%
38	21.877	3194	3198	3202	rBV3	41810	63527	3.26%	0.539%
39	22.112	3231	3238	3243	rBV10	12012	29916	1.53%	0.254%
40	22.418	3288	3290	3296	rVB	19905	26748	1.37%	0.227%
41	22.488	3297	3302	3312	rVB2	58736	109433	5.61%	0.929%
42	23.188	3415	3421	3429	rVB2	61942	125574	6.43%	1.066%
43	23.893	3535	3541	3550	rBV3	46986	147235	7.54%	1.250%
44	23.998	3555	3559	3568	rVB2	54261	119077	6.10%	1.011%
45	24.621	3657	3665	3673	rBV3	28144	77066	3.95%	0.654%
46	24.768	3683	3690	3698	rVB	36349	98088	5.03%	0.833%
47	24.921	3706	3716	3736	rBV2	298845	979733	50.20%	8.316%
48	26.096	3910	3916	3930	rVB4	25766	75935	3.89%	0.645%

Sum of corrected areas: 11780993

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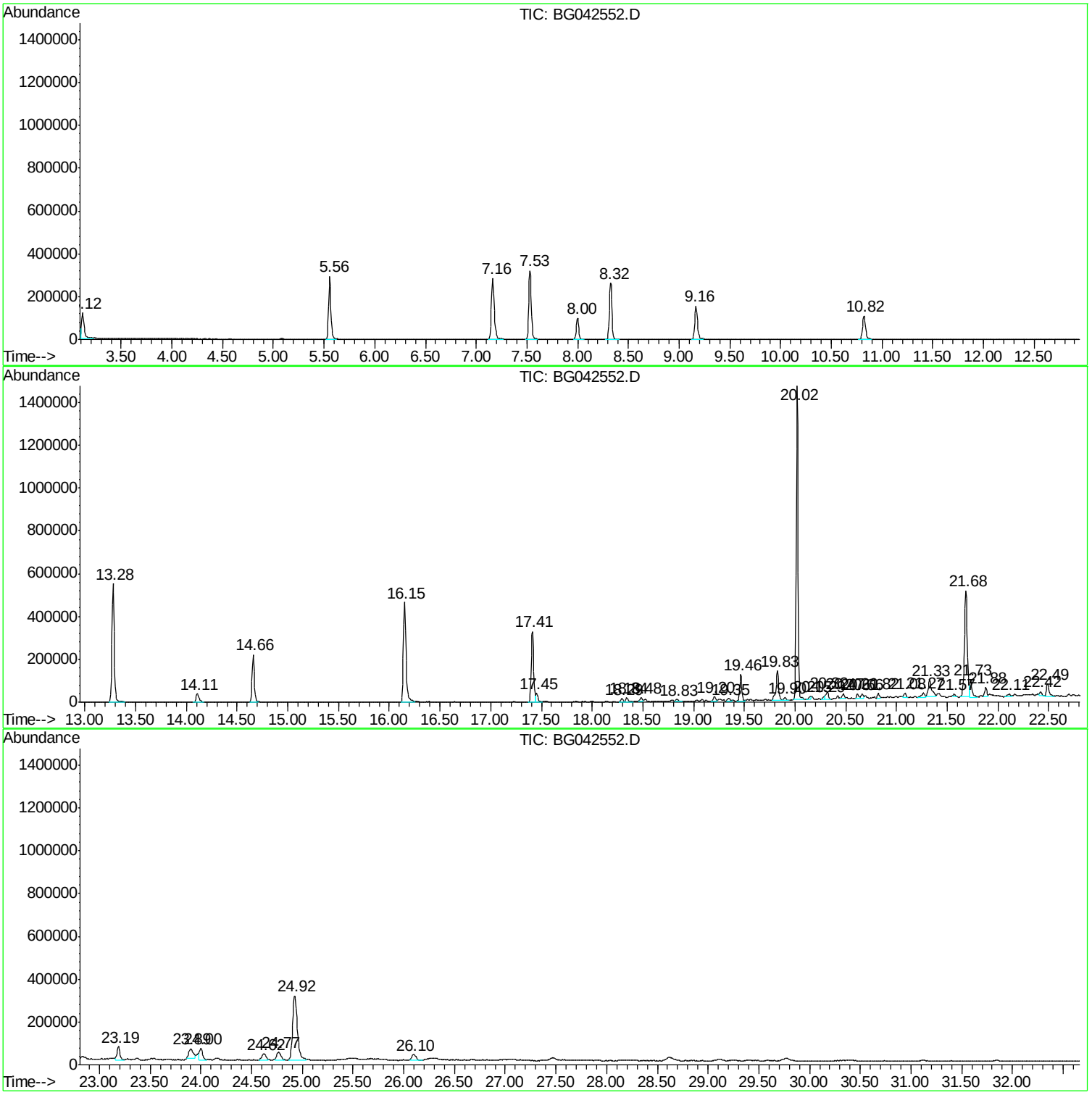
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

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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Data File : BG042552.D
Acq On : 29 Aug 2019 3:57
Operator : HP/JU
Sample : K4543-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

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

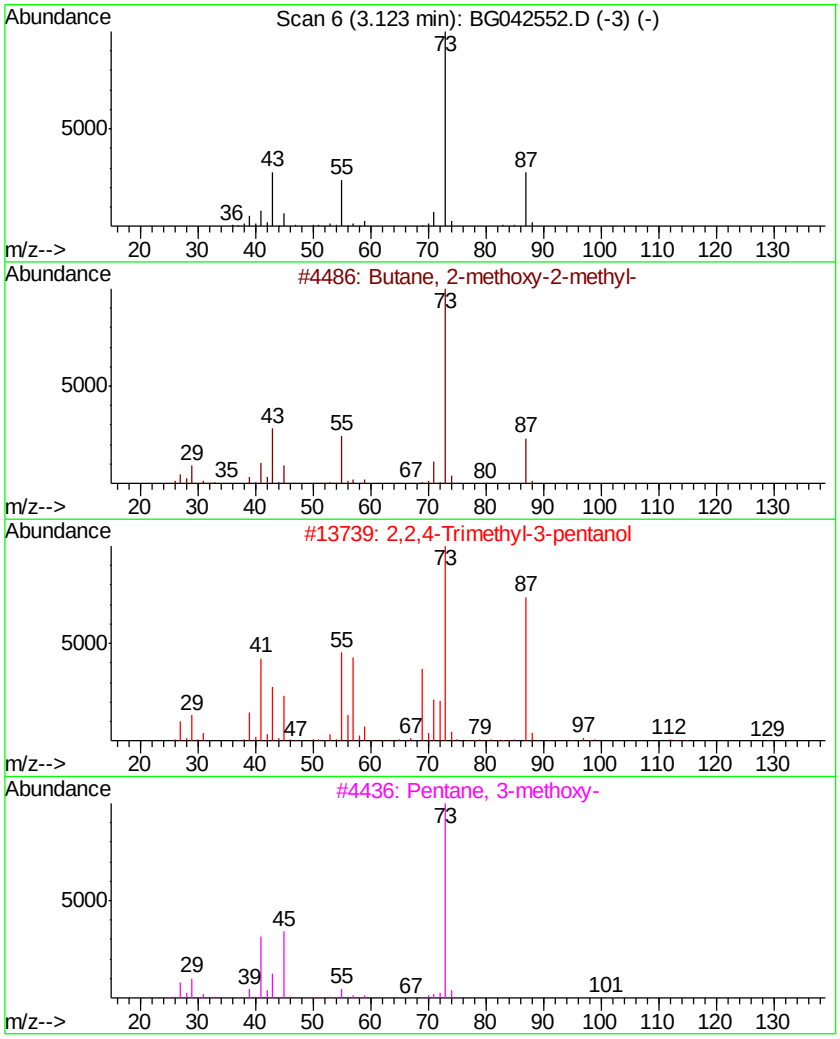
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

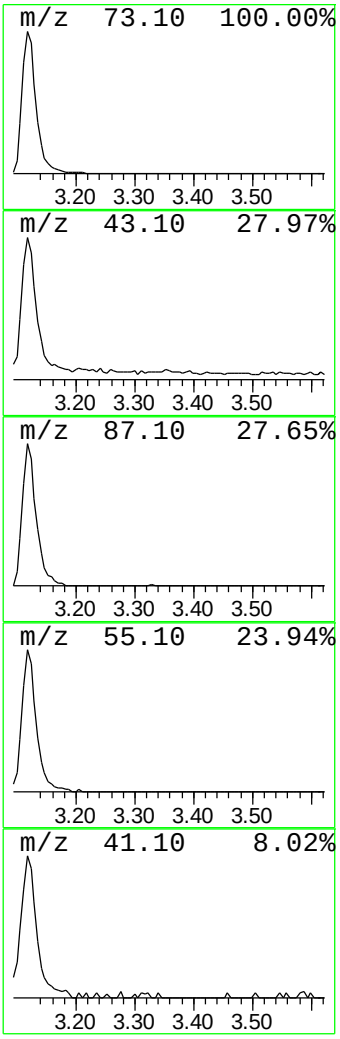
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	21.69 ng	186567	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042552.D
Acq On : 29 Aug 2019 3:57
Operator : HP/JU
Sample : K4543-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

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

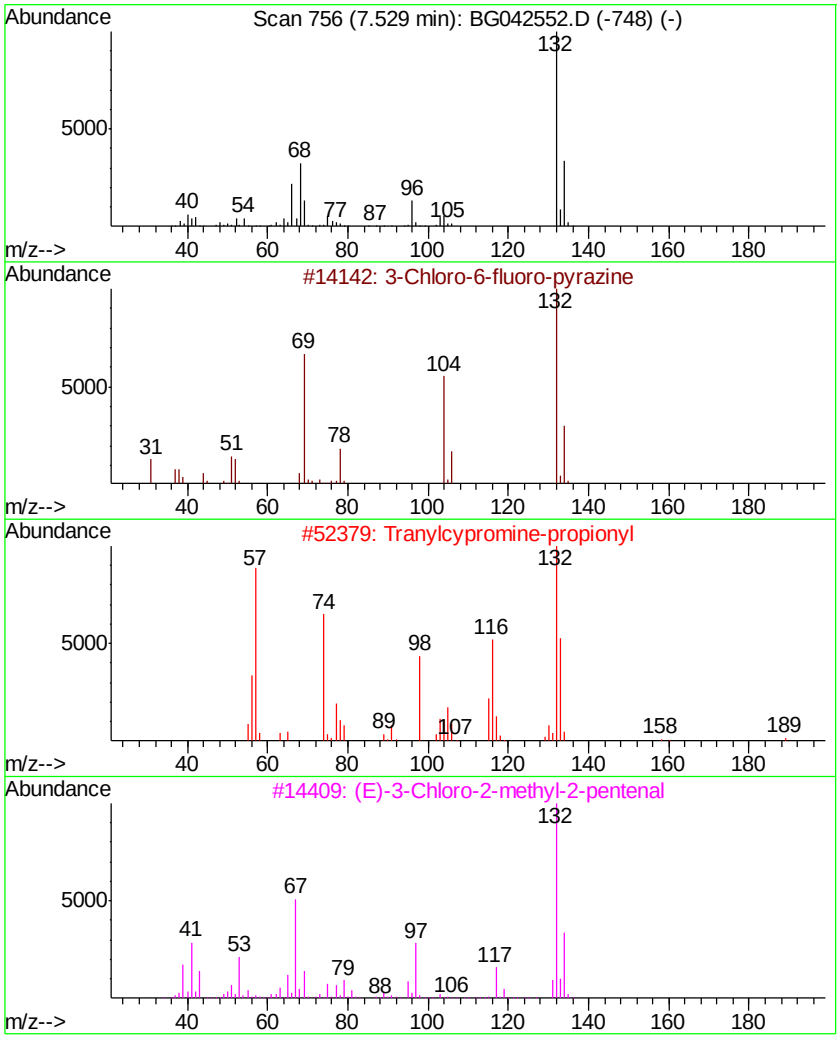
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

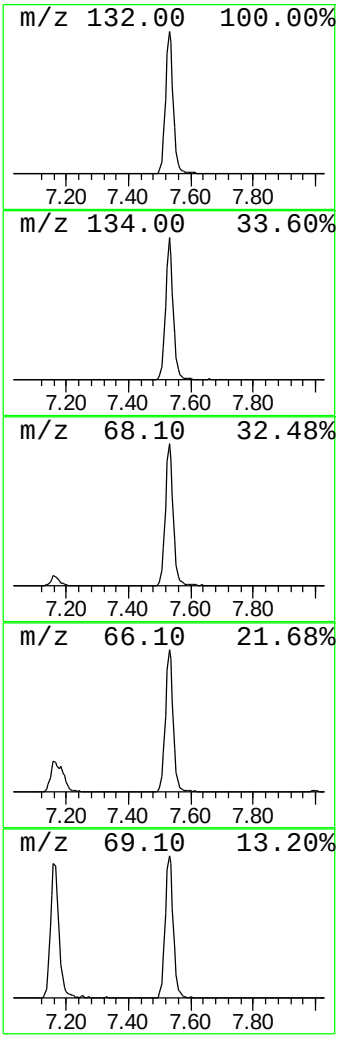
****

Peak Number 2 unknown7.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	65.75 ng	565498	1,4-Dichlorobenzene-d4	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042552.D
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Operator : HP/JU
Sample : K4543-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

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

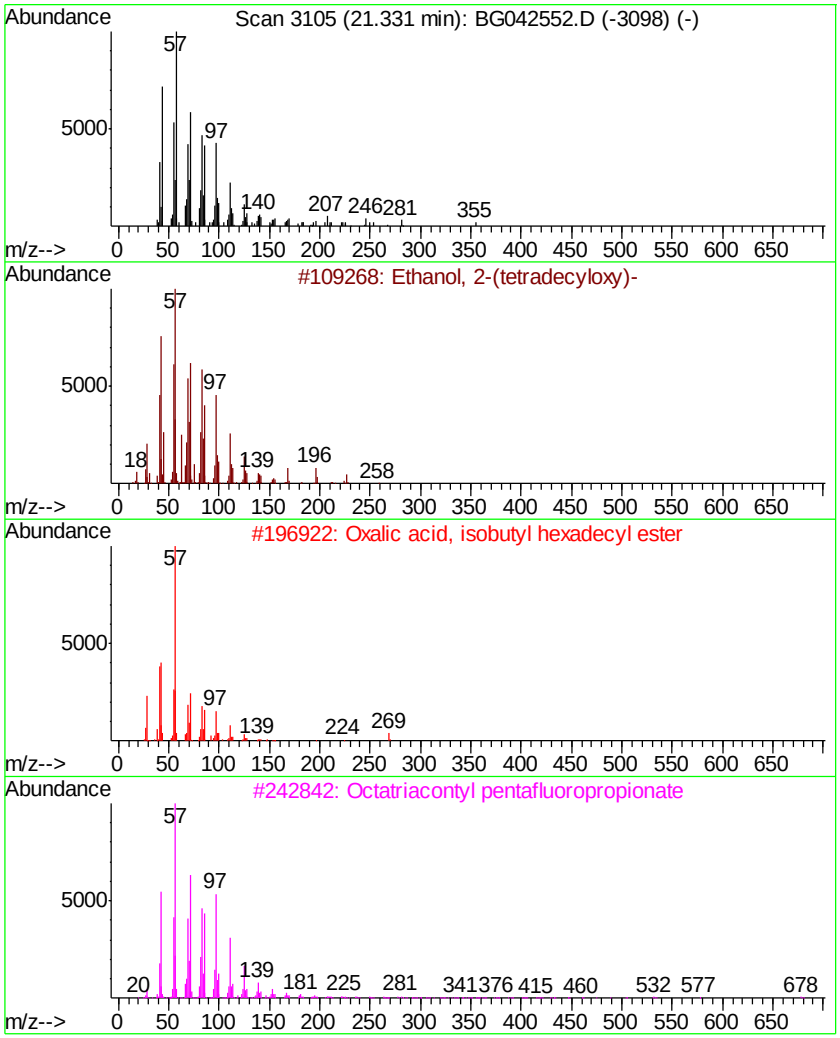
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

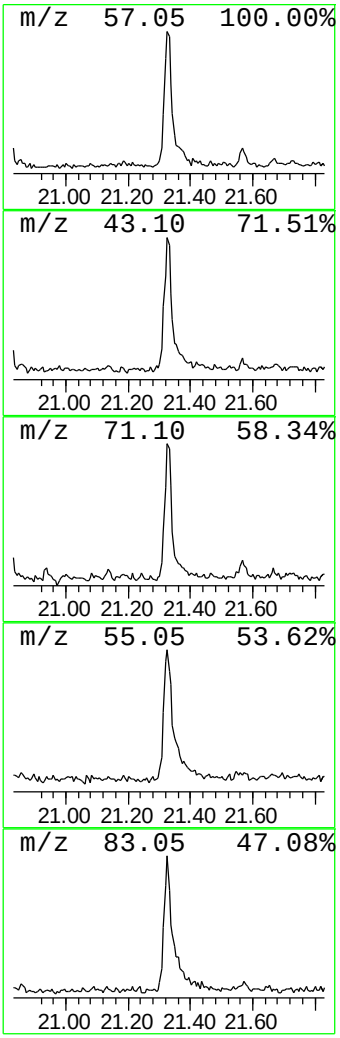
****

Peak Number 4 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	3.69 ng	178100	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	87
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
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Sample : K4543-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

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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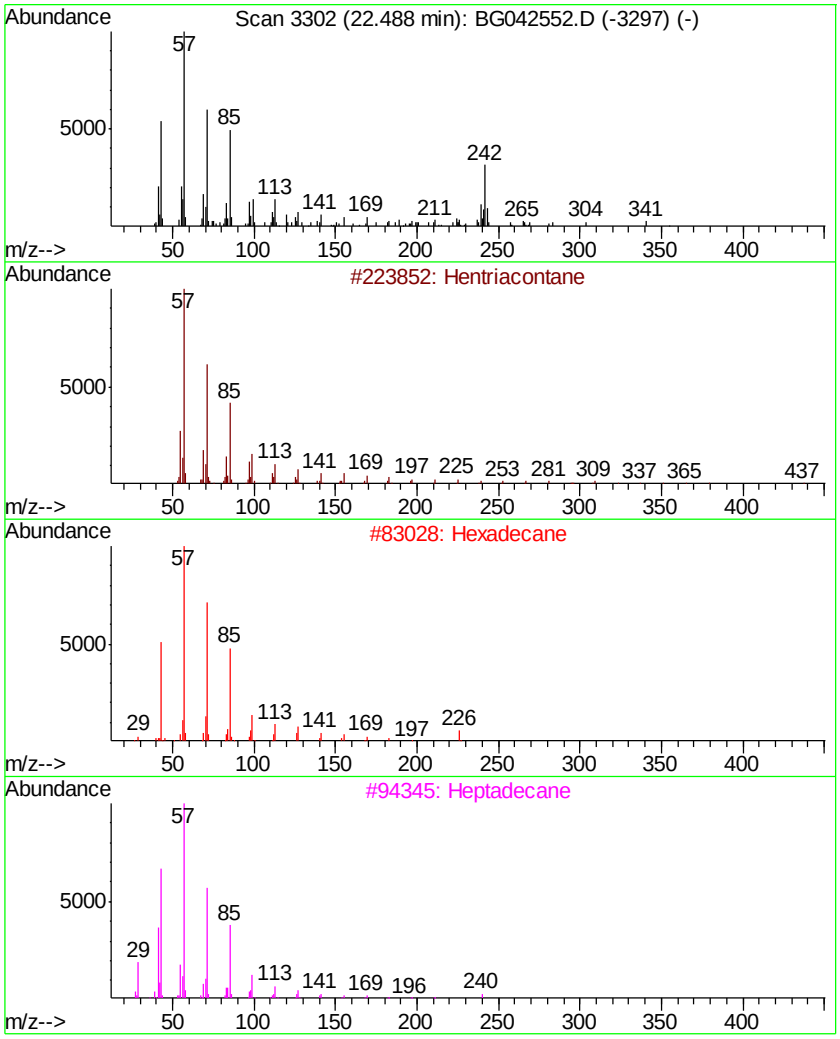
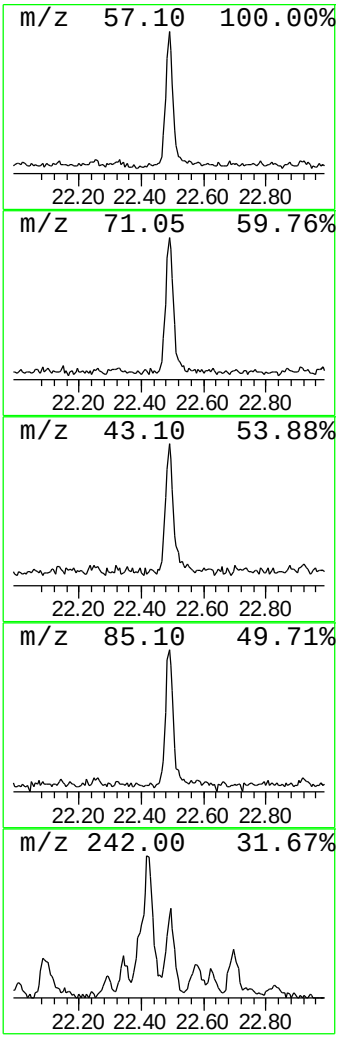
Peak Number 5 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	2.27 ng	109433	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	87
2	Hexadecane	226	C16H34	000544-76-3	83
3	Heptadecane	240	C17H36	000629-78-7	83
4	Triacontane	422	C30H62	000638-68-6	70
5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	68





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : TP-3-S

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

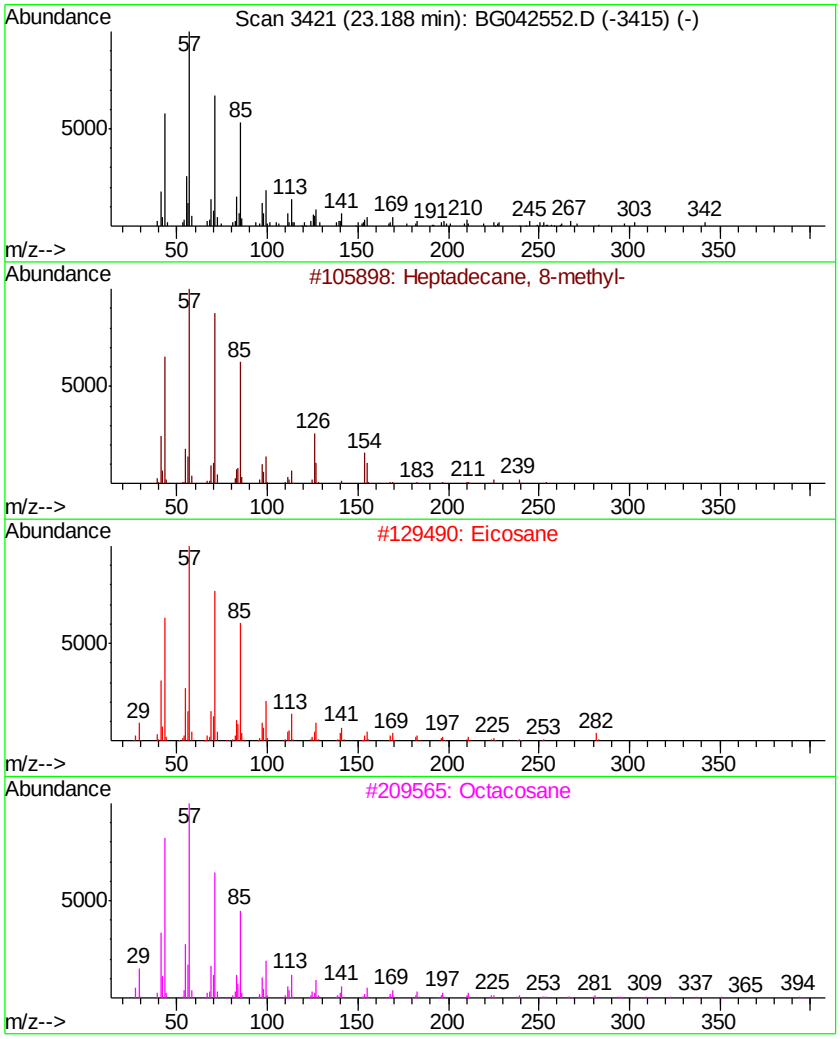
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

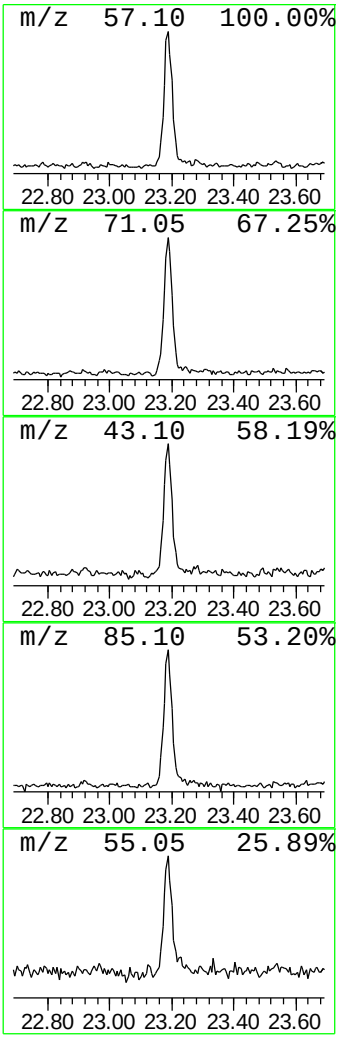
****

Peak Number 6 Heptadecane, 8-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	2.60 ng	125574	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	93
2	Eicosane	282	C20H42	000112-95-8	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Heneicosane	296	C21H44	000629-94-7	90





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Misc :
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Instrument : BNA_G
ClientSampleId : TP-3-S

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

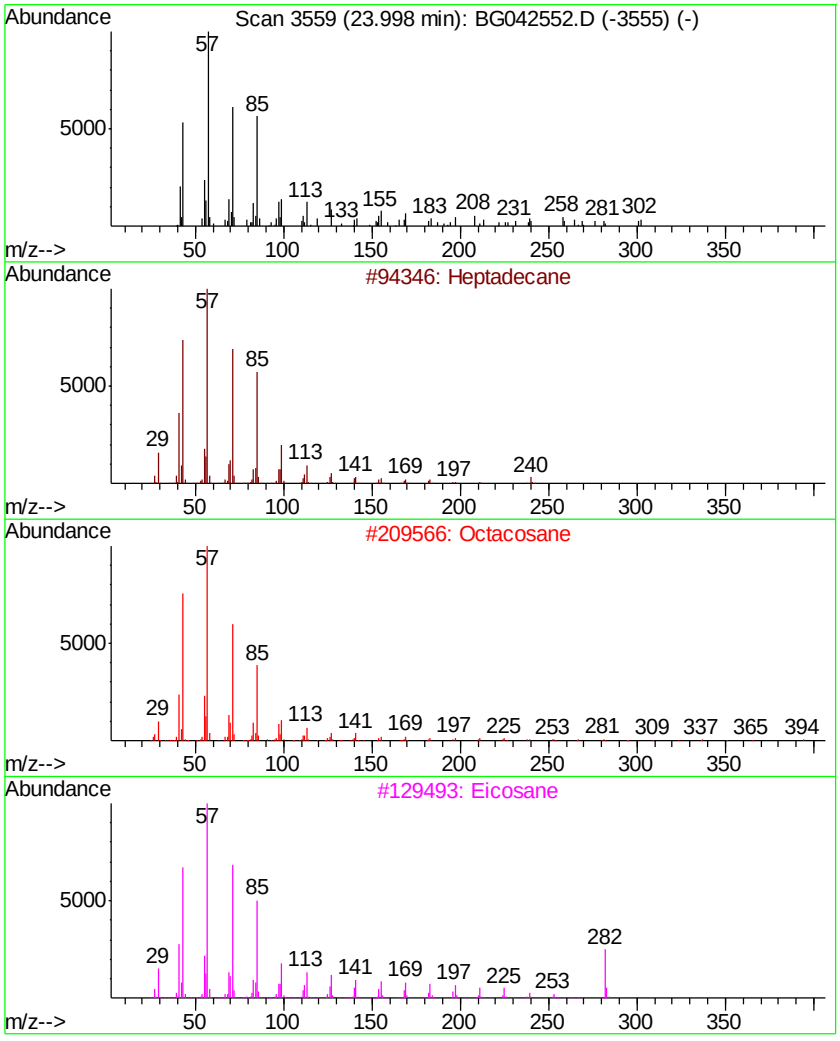
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

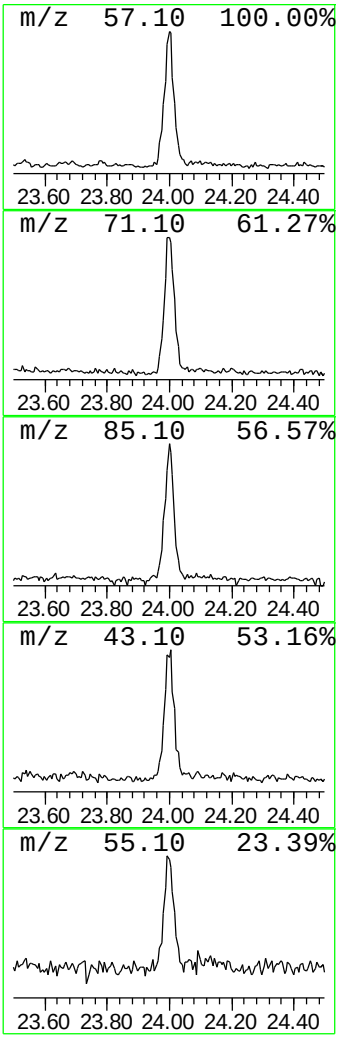
****

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	2.43 ng	119077	Perylene-d12	24.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Octacosane	394	C28H58	000630-02-4	83
3	Eicosane	282	C20H42	000112-95-8	81
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
5	Pentacosane	352	C25H52	000629-99-2	72





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	186567	1	8.00	172010	20.0
unknown7.53	7.53	65.8	ng	565498	1	8.00	172010	20.0
Ethanol, 2-(tetra...	21.33	3.7	ng	178100	5	21.68	966240	20.0
Hentriacontane	22.49	2.3	ng	109433	5	21.68	966240	20.0
Heptadecane, 8-me...	23.19	2.6	ng	125574	5	21.68	966240	20.0
Heptadecane	24.00	2.4	ng	119077	6	24.92	979733	20.0