LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042548.D
Acq On : 29 Aug 2019 1:06
Operator : HP/JU
Sample : K4571-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200052

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	23	rVB	391485	484447	21.39%	3.674%
2	5.555	413	420	432	rBV	317238	534871	23.62%	4.057%
3	7.159	684	693	710	rBV	325132	640516	28.28%	4.858%
4	7.530	749	756	767	rBV	362979	629969	27.82%	4.778%
5	8.000	828	836	845	rBV	93805	157034	6.93%	1.191%
6	8.323	884	891	904	rVB	284345	488090	21.55%	3.702%
7	9.169	1027	1035	1047	rBV	178741	360012	15.90%	2.731%
8	10.820	1308	1316	1333	rBV	113004	233681	10.32%	1.772%
9	13.276	1727	1734	1757	rBV	657012	1068331	47.18%	8.103%
10	14.104	1870	1875	1884	rBV	37621	67225	2.97%	0.510%
11	14.657	1961	1969	1975	rBV	248551	407793	18.01%	3.093%
12	14.721	1975	1980	1990	rVB	107839	174235	7.69%	1.322%
13	15.062	2031	2038	2047	rBV	40521	70524	3.11%	0.535%
14	15.708	2141	2148	2158	rBV	64144	104244	4.60%	0.791%
15	16.149	2216	2223	2244	rBV	653825	1160843	51.26%	8.805%
16	16.384	2258	2263	2273	rVB5	14606	28565	1.26%	0.217%
17	17.230	2402	2407	2416	rVB	15892	25221	1.11%	0.191%
18	17.412	2431	2438	2442	rBV	387551	620827	27.42%	4.709%
19	17.453	2442	2445	2453	rVV	180676	267629	11.82%	2.030%
20	17.541	2453	2460	2467	rVB3	27907	58646	2.59%	0.445%
21	18.487	2615	2621	2626	rBV2	36557	62761	2.77%	0.476%
22	19.463	2782	2787	2794	rBV	195050	290694	12.84%	2.205%
23	19.827	2839	2849	2857	rBV	147361	273919	12.10%	2.078%
24	20.021	2876	2882	2892	rBV	1694629	2264551	100.00%	17.176%
25	20.321	2925	2933	2938	rBV2	31231	52828	2.33%	0.401%
26	20.420	2945	2950	2953	rBV2	18460	25083	1.11%	0.190%
27	20.820	3014	3018	3022	rBV2	30322	35270	1.56%	0.268%
28	21.325	3098	3104	3117	rBV4	109037	233389	10.31%	1.770%
29	21.684	3157	3165	3172	rBV2	470681	860420	38.00%	6.526%
30	21.878	3193	3198	3205	rVB3	51758	80823	3.57%	0.613%
31	22.489	3297	3302	3307	rBV2	55342	97178	4.29%	0.737%
32	22.865	3361	3366	3373	rBV4	23159	41344	1.83%	0.314%
33	23.188	3415	3421	3428	rBV2	63586	120979	5.34%	0.918%
34	23.999	3553	3559	3572	rVB2	50322	116228	5.13%	0.882%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042548.D
Acq On : 29 Aug 2019 1:06
Operator : HP/JU
Sample : K4571-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200052

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	24.927	3705	3717	3737	rBV2	299563	976547	43.12%	7.407%
36	26.096	3909	3916	3930	rVB3	21403	69327	3.06%	0.526%

Sum of corrected areas: 13184044

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
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Acq On : 29 Aug 2019 1:06
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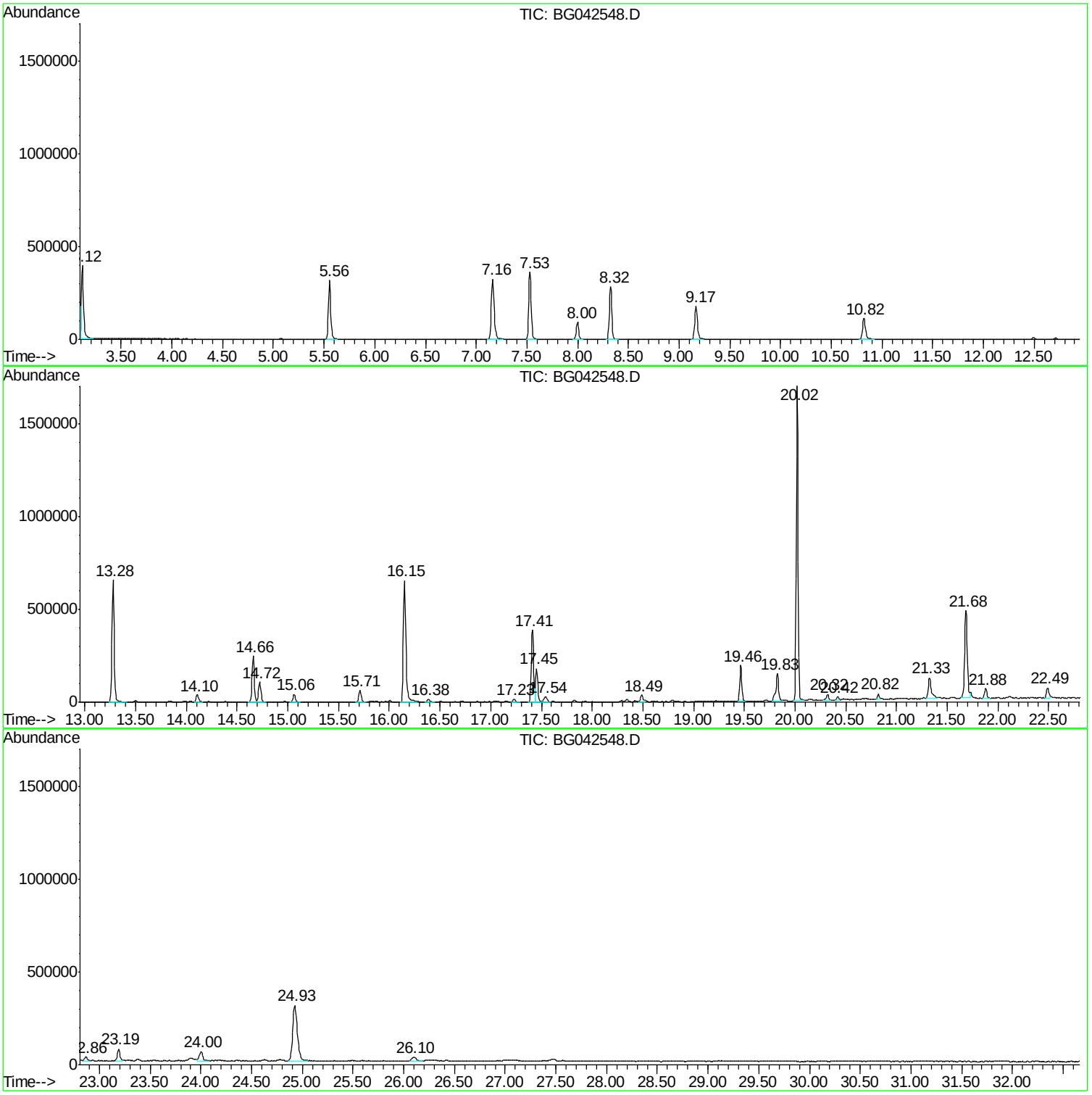
Sample : K4571-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200052

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042548.D
Acq On : 29 Aug 2019 1:06
Operator : HP/JU
Sample : K4571-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200052

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

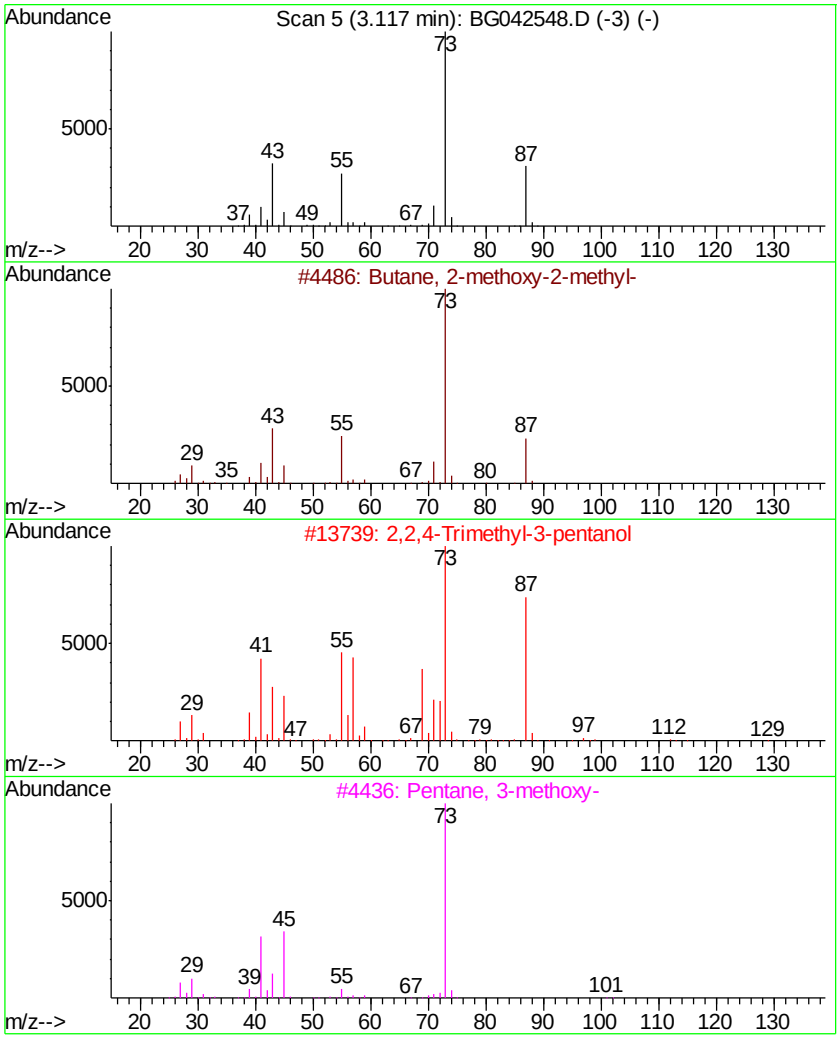
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

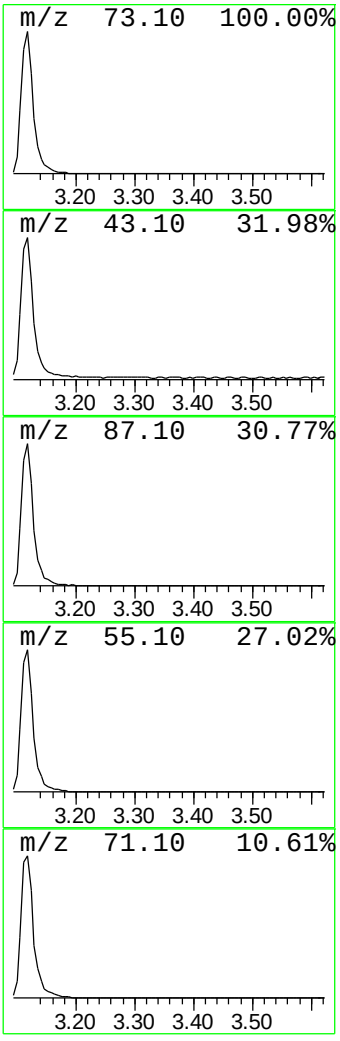
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	61.70 ng	484447	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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042548.D
Acq On : 29 Aug 2019 1:06
Operator : HP/JU
Sample : K4571-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200052

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

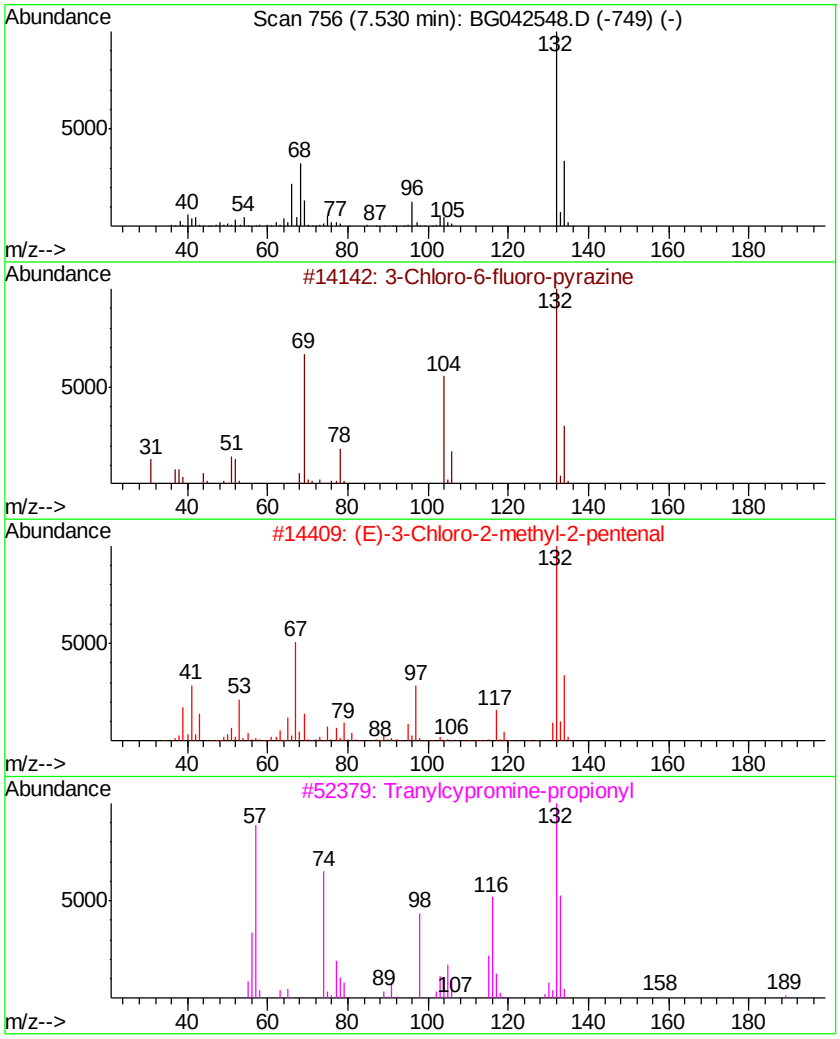
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

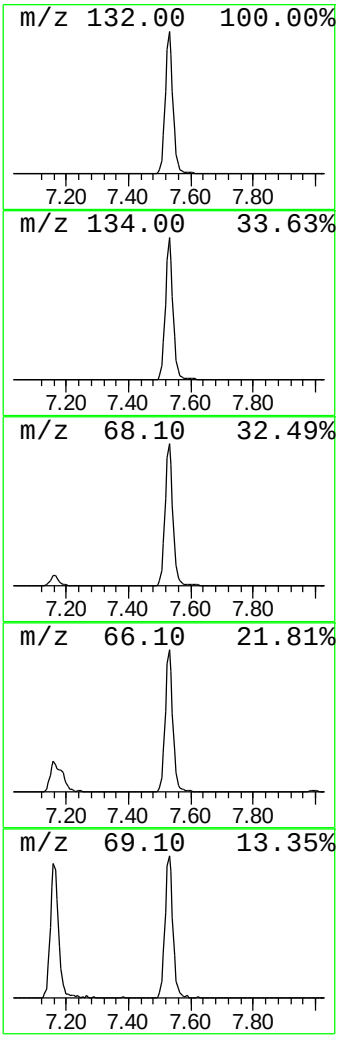
****

Peak Number 2 unknown7.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	80.23 ng	629969	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042548.D
Acq On : 29 Aug 2019 1:06
Operator : HP/JU
Sample : K4571-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200052

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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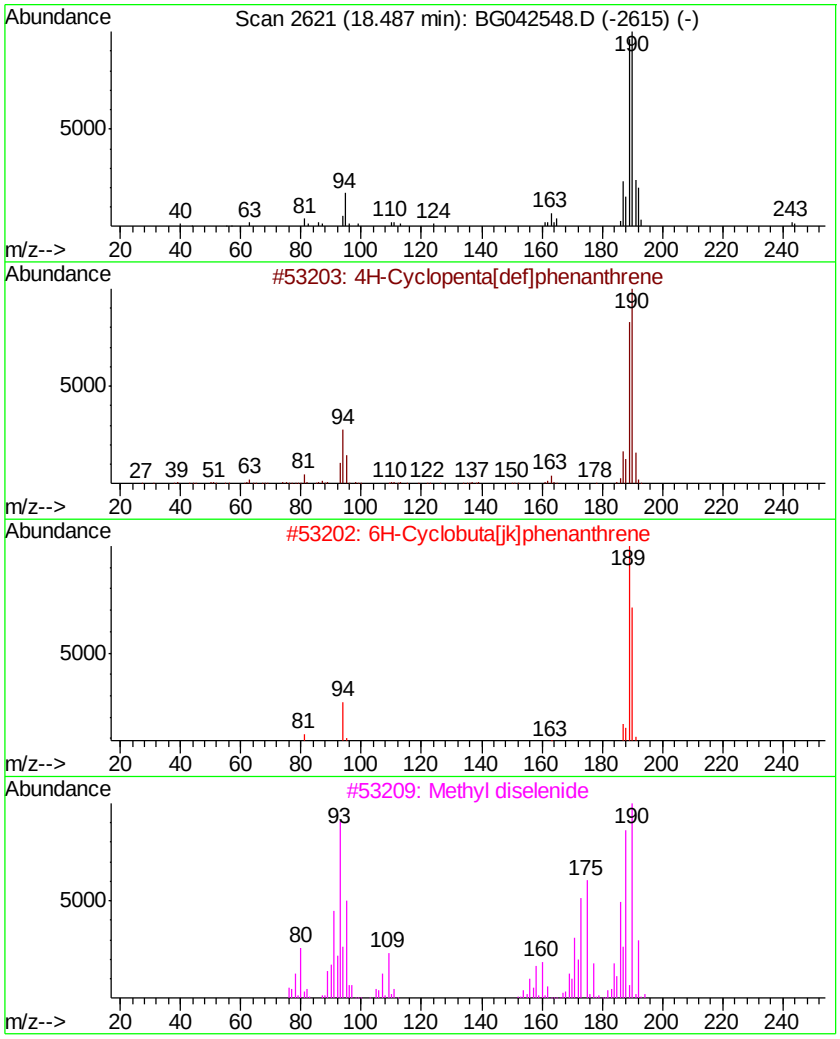
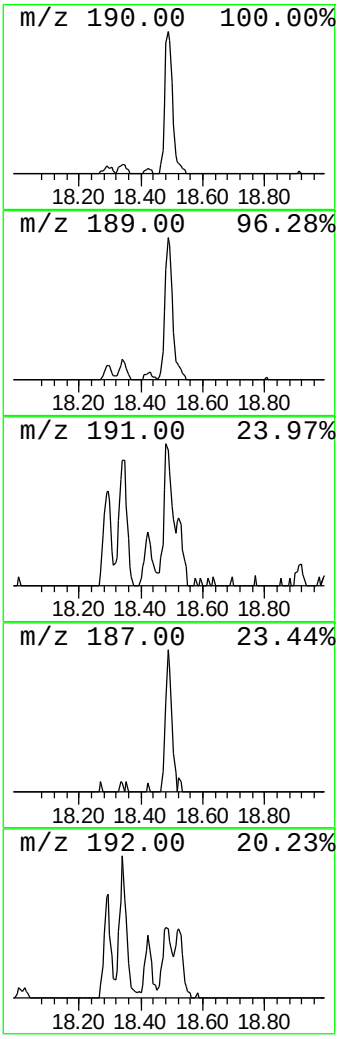
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.49	2.02 ng	62761	Phenanthrene-d10	17.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	Methyl diselenide	190	C2H6Se2	007101-31-7	55
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042548.D
Acq On : 29 Aug 2019 1:06
Operator : HP/JU
Sample : K4571-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200052

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

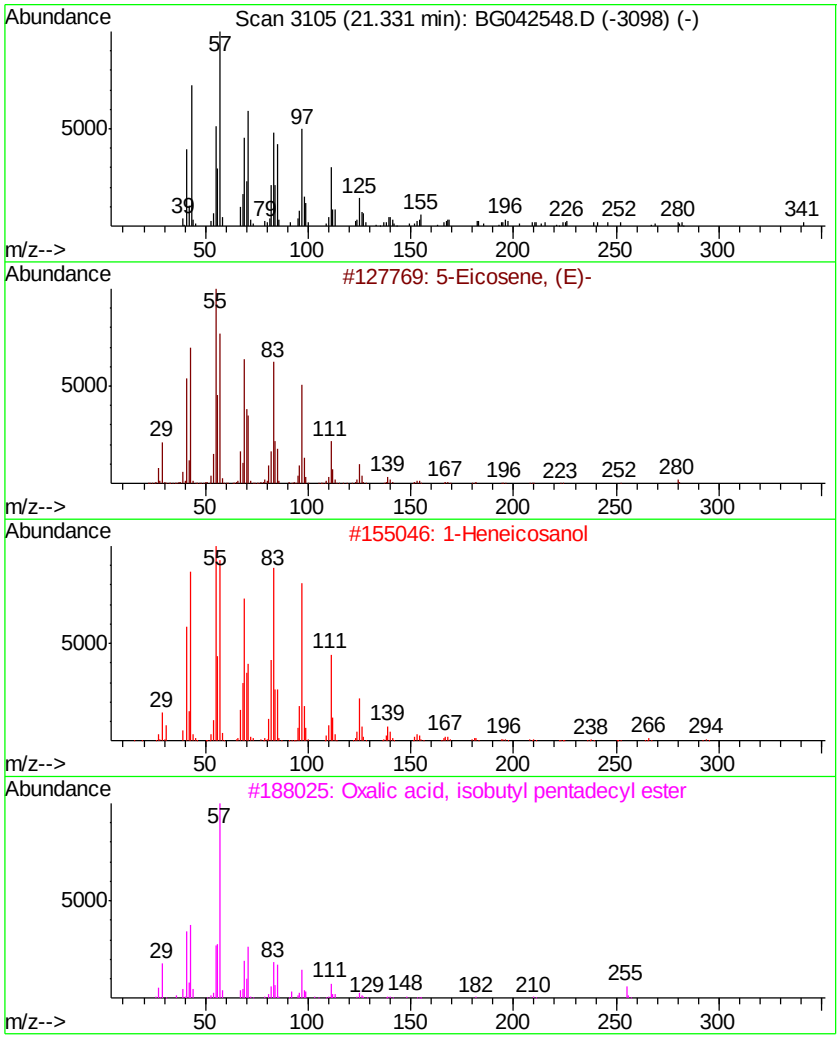
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

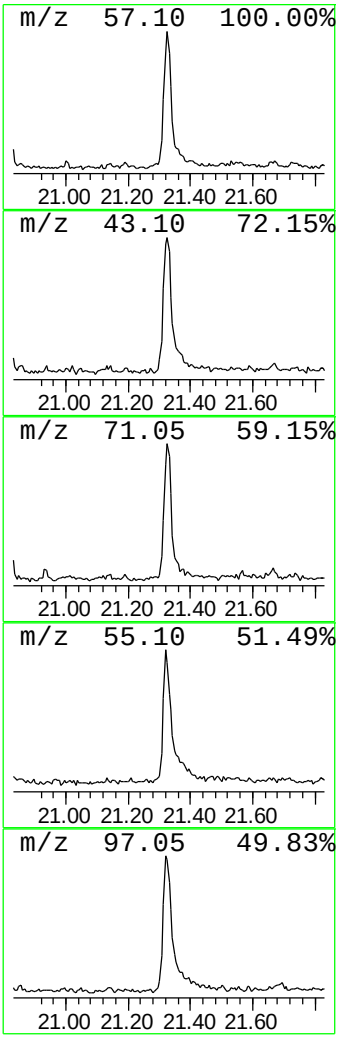
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	5.43 ng	233389	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	92
3	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
5	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082819\
Data File : BG042548.D
Acq On : 29 Aug 2019 1:06
Operator : HP/JU
Sample : K4571-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-200052

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

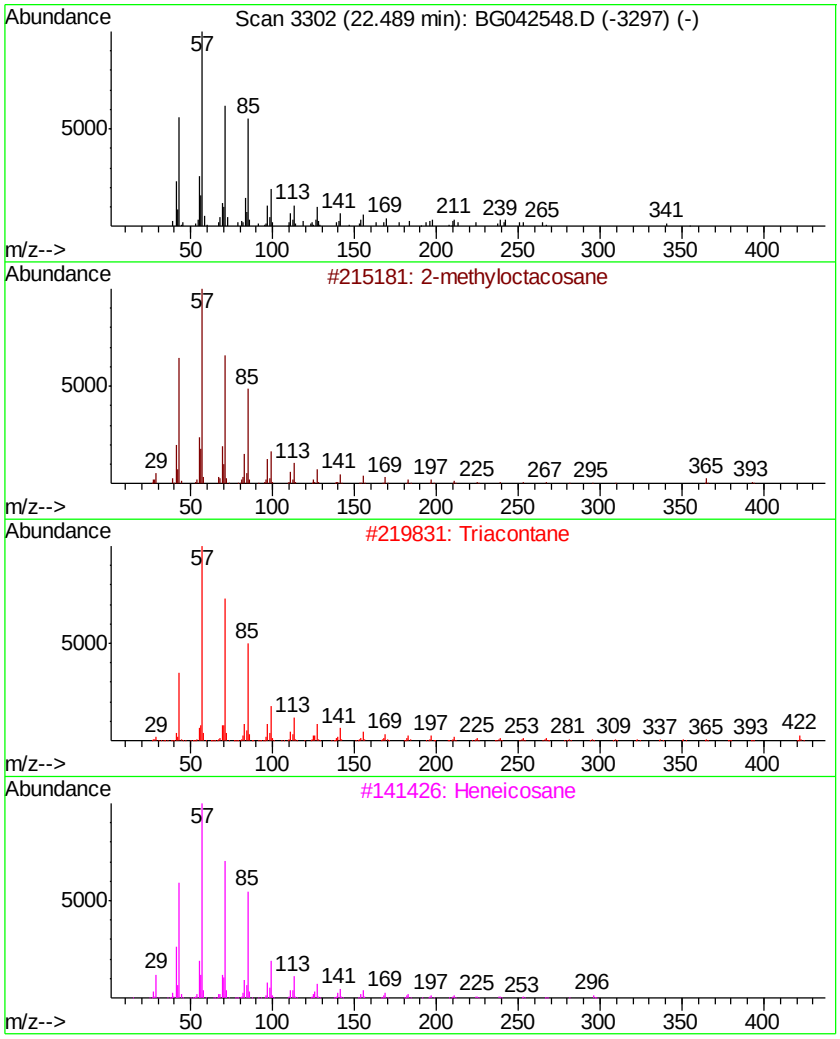
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

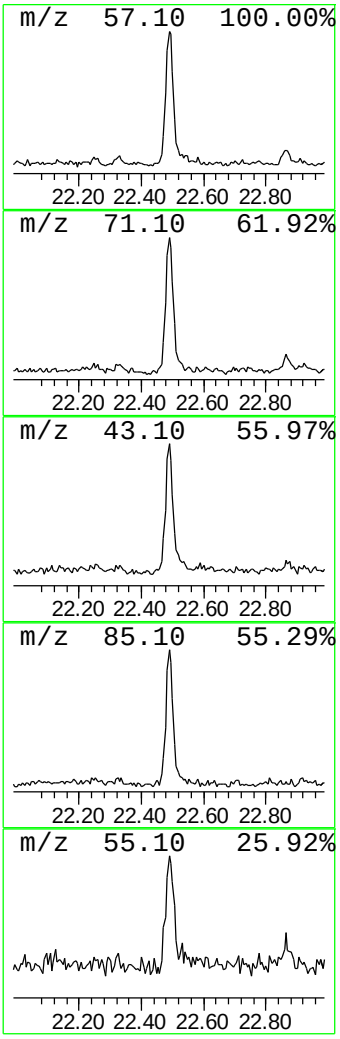
****

Peak Number 6 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	2.26 ng	97178	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Octacosane	394	C28H58	000630-02-4	91





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Misc :
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Instrument : BNA_G
ClientSampleId : RBR-200052

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

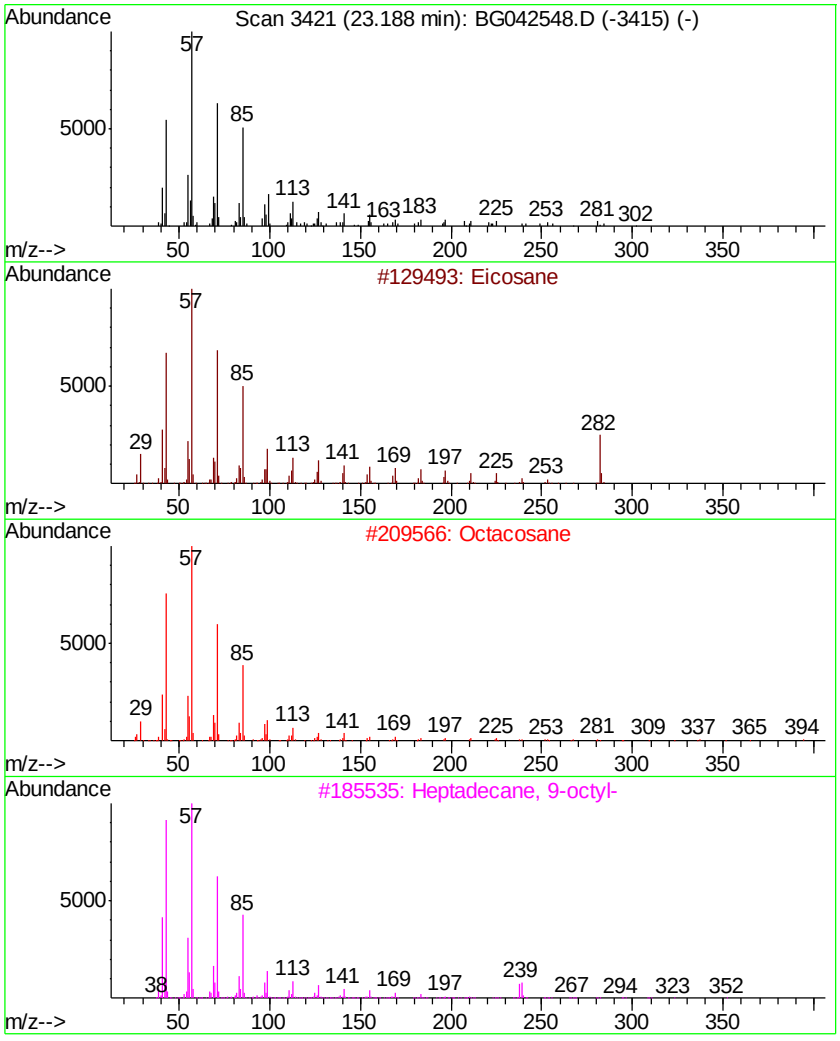
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

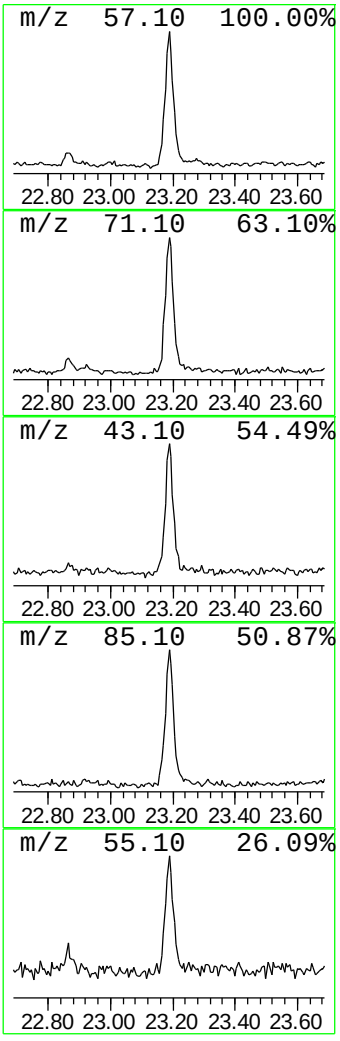
****

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	2.81 ng	120979	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Triacontane	422	C30H62	000638-68-6	90





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : RBR-200052

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

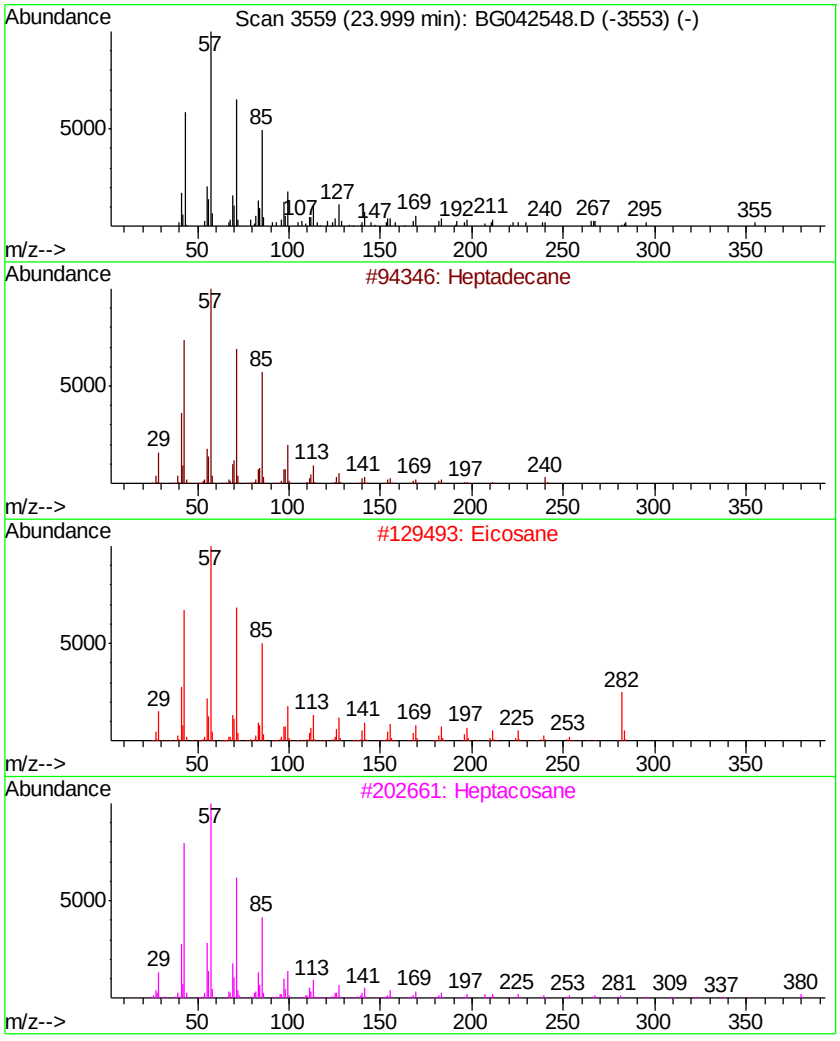
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

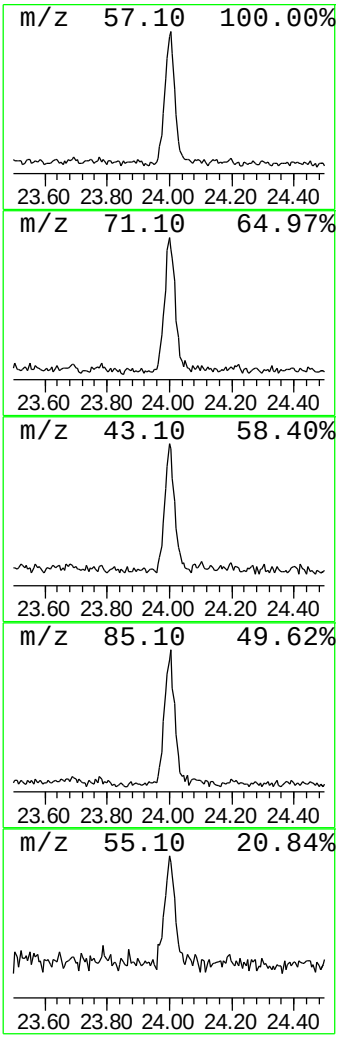
****

Peak Number 8 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	2.38 ng	116228	Perylene-d12	24.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	95
2	Eicosane	282	C20H42	000112-95-8	93
3	Heptacosane	380	C27H56	000593-49-7	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG082819\
Data File : BG042548.D
Acq On : 29 Aug 2019 1:06
Operator : HP/JU
Sample : K4571-07
Misc :
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Instrument : BNA_G
ClientSampleId : RBR-200052

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.12	61.7	ng	484447	1	8.00	157034	20.0
unknown7.53	7.53	80.2	ng	629969	1	8.00	157034	20.0
4H-Cyclopenta[def...	18.49	2.0	ng	62761	4	17.41	620827	20.0
5-Eicosene, (E)-	21.33	5.4	ng	233389	5	21.68	860420	20.0
2-methyloctacosane	22.49	2.3	ng	97178	5	21.68	860420	20.0
Eicosane	23.19	2.8	ng	120979	5	21.68	860420	20.0
Heptadecane	24.00	2.4	ng	116228	6	24.93	976547	20.0