LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-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:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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	3.385	10	16	18	rBV5	24696	43257	2.41%	0.361%
2	3.473	25	31	46	rVB	444629	738700	41.16%	6.166%
3	6.158	481	488	500	rBV	123721	217874	12.14%	1.819%
4	7.833	767	773	786	rBV4	90550	227145	12.66%	1.896%
5	8.238	834	842	856	rVB	285033	515195	28.71%	4.300%
6	8.726	918	925	938	rVB	131179	262687	14.64%	2.193%
7	9.061	974	982	995	rVB	252471	470206	26.20%	3.925%
8	9.924	1120	1129	1138	rBV	195605	378805	21.11%	3.162%
9	11.605	1407	1415	1427	rVB	188675	363299	20.24%	3.033%
10	13.984	1810	1820	1830	rVB	785298	1272135	70.88%	10.619%
11	14.519	1907	1911	1916	rBV5	11845	19776	1.10%	0.165%
12	14.783	1950	1956	1962	rBV	123354	186412	10.39%	1.556%
13	14.983	1987	1990	1994	rVB4	16032	22989	1.28%	0.192%
14	15.201	2022	2027	2031	rBV2	39254	52408	2.92%	0.437%
15	15.359	2048	2054	2064	rVB2	338033	581270	32.39%	4.852%
16	15.817	2124	2132	2133	rBV4	14027	20627	1.15%	0.172%
17	15.882	2139	2143	2148	rVB4	13383	19666	1.10%	0.164%
18	16.141	2183	2187	2193	rVB2	56868	80007	4.46%	0.668%
19	16.546	2247	2256	2260	rBV7	11635	27390	1.53%	0.229%
20	16.834	2298	2305	2314	rBV	687914	1122247	62.53%	9.368%
21	16.910	2315	2318	2324	rVB7	18487	25036	1.39%	0.209%
22	16.998	2328	2333	2344	rBV4	52303	108377	6.04%	0.905%
23	17.345	2387	2392	2399	rBV2	16062	28044	1.56%	0.234%
24	17.474	2406	2414	2419	rVB5	27658	47971	2.67%	0.400%
25	17.786	2462	2467	2472	rBV4	29458	47450	2.64%	0.396%
26	17.833	2472	2475	2480	rVB5	13848	23303	1.30%	0.195%
27	18.091	2512	2519	2527	rBV2	446083	738000	41.12%	6.160%
28	18.914	2653	2659	2668	rBV2	131485	214390	11.95%	1.790%
29	19.002	2668	2674	2678	rVB2	10984	24867	1.39%	0.208%
30	19.149	2693	2699	2705	rVB10	15776	28077	1.56%	0.234%
31	19.513	2757	2761	2766	rVB8	12519	19845	1.11%	0.166%
32	20.083	2855	2858	2863	rVV5	20503	21813	1.22%	0.182%
33	20.148	2866	2869	2876	rVV4	42639	60219	3.36%	0.503%
34	20.630	2945	2951	2961	rBV	1304810	1794732	100.00%	14.981%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-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:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.969	3174	3179	3190	rBV4	80383	182210	10.15%	1.521%
36	22.427	3248	3257	3265	rBV2	516266	977764	54.48%	8.162%
37	24.290	3567	3574	3585	rVB5	19532	44249	2.47%	0.369%
38	26.117	3873	3885	3899	rBV2	272524	971611	54.14%	8.110%

Sum of corrected areas: 11980053

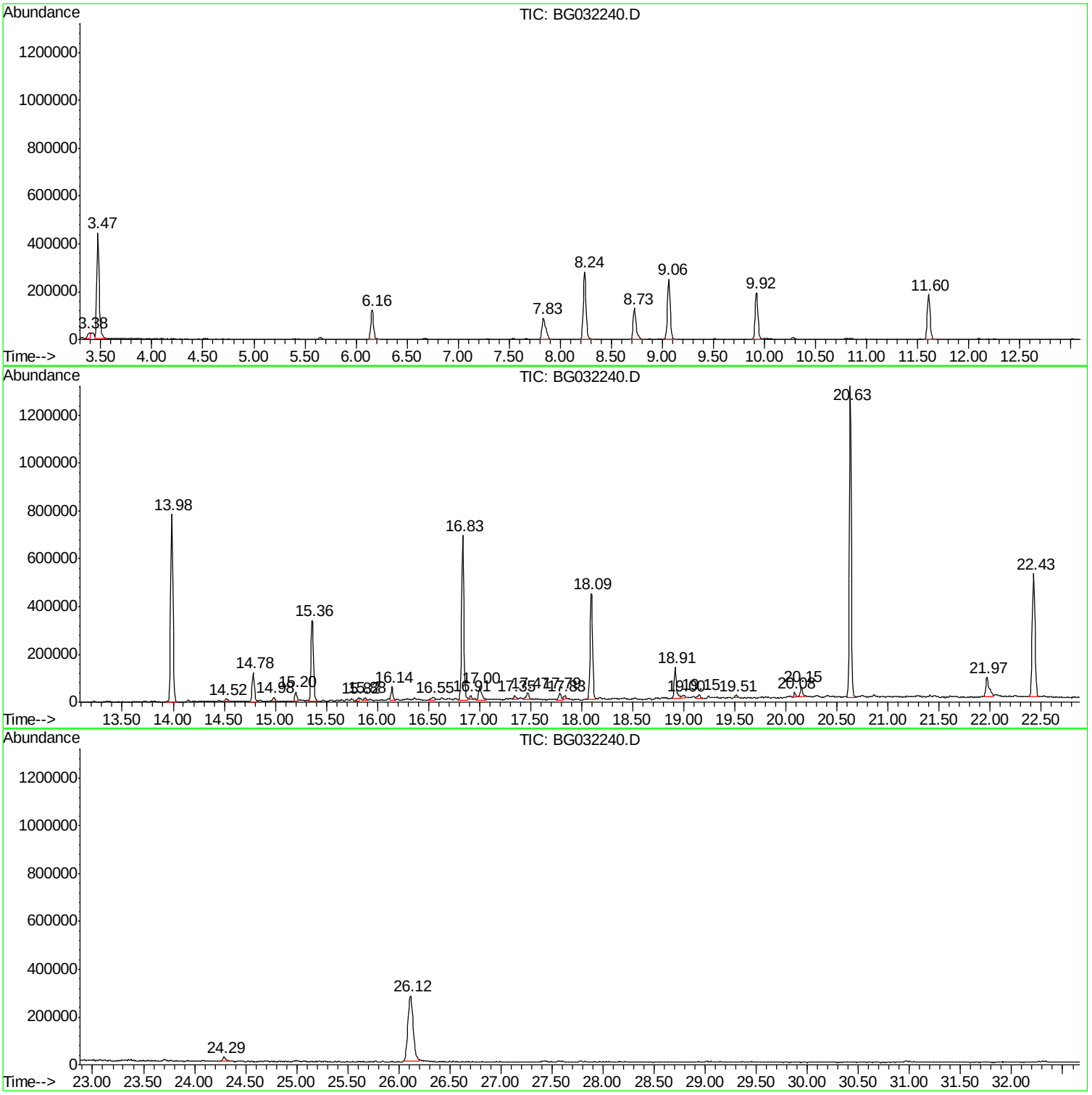
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

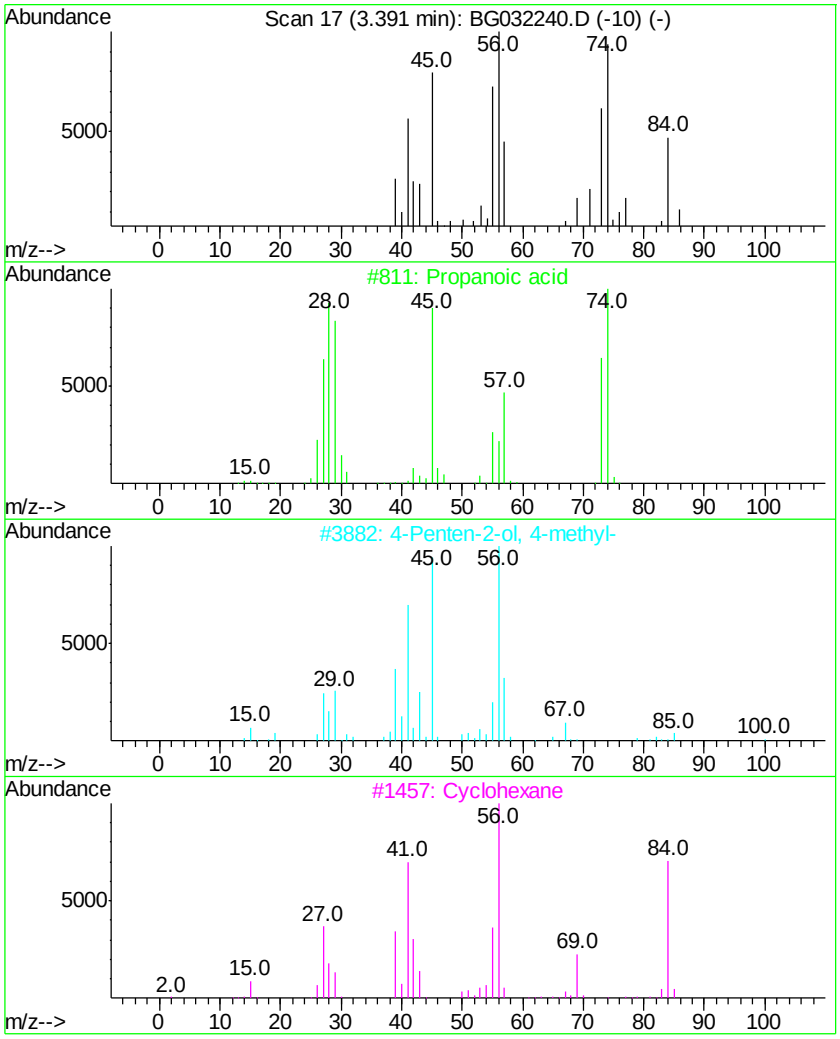
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

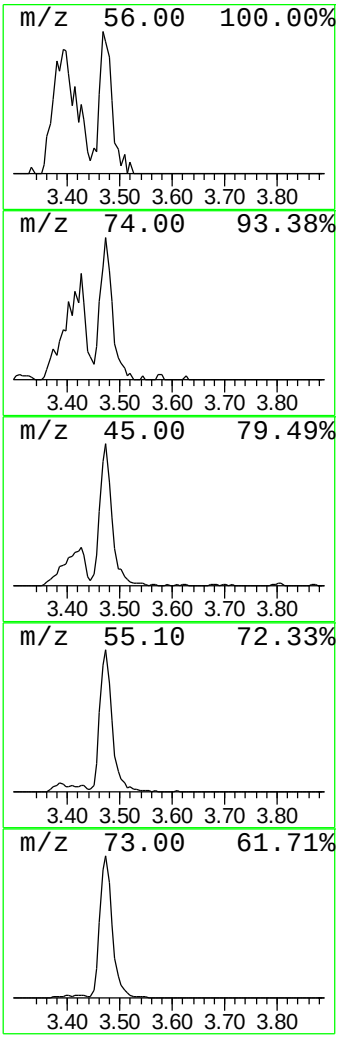
****

Peak Number 1 unknown3.39 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.39	3.29 ng	43257	1,4-Dichlorobenzene-d4	8.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid	74	C3H6O2	000079-09-4	43
2	4-Penten-2-ol, 4-methyl-	100	C6H12O	002004-67-3	35
3	Cyclohexane	84	C6H12	000110-82-7	18
4	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	14
5	Hexane, 2-chloro-	120	C6H13Cl	000638-28-8	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

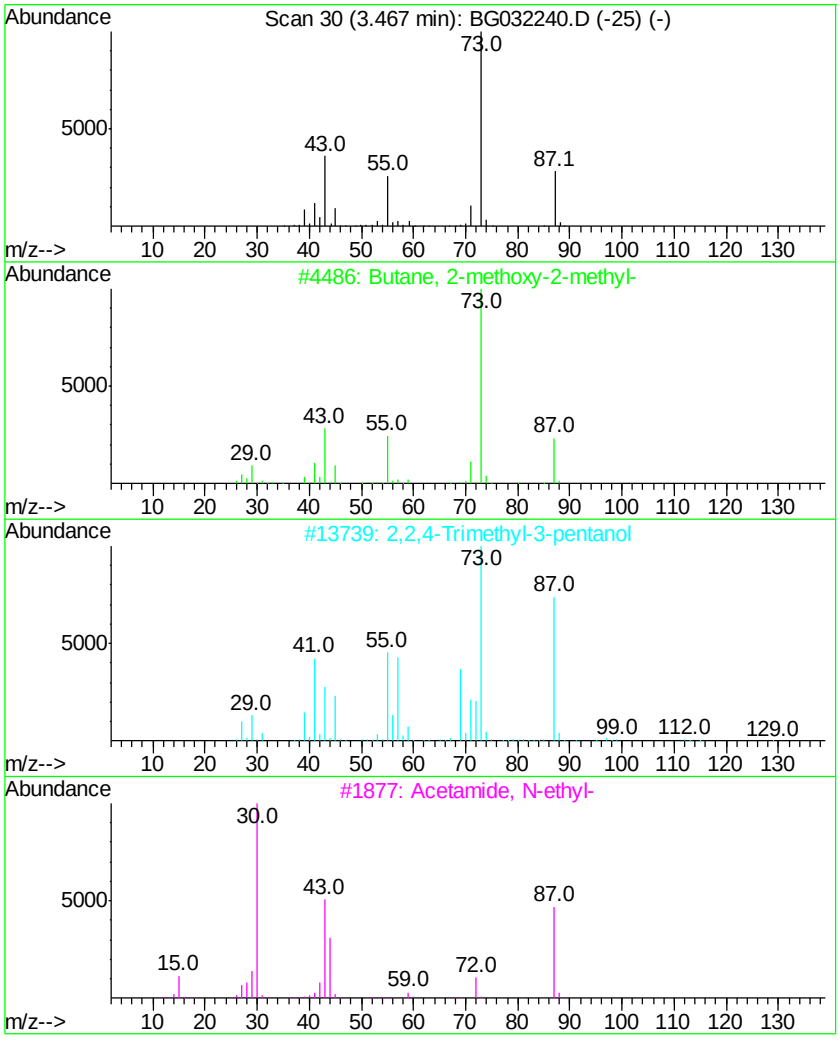
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

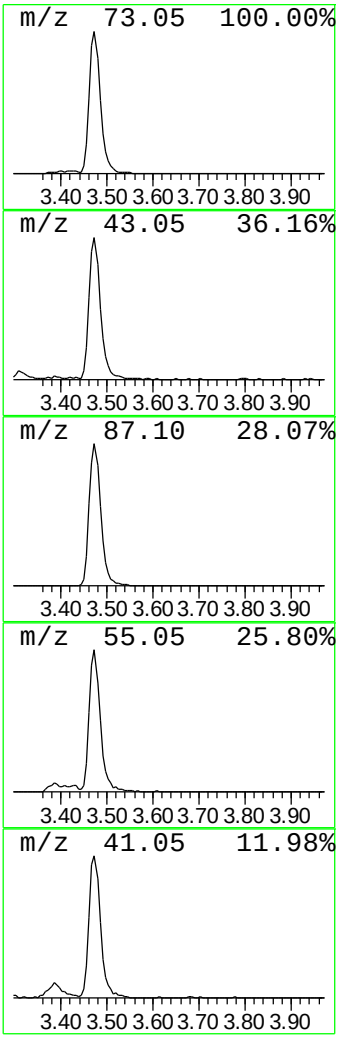
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.47	56.24 ng	738700	1,4-Dichlorobenzene-d4	8.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

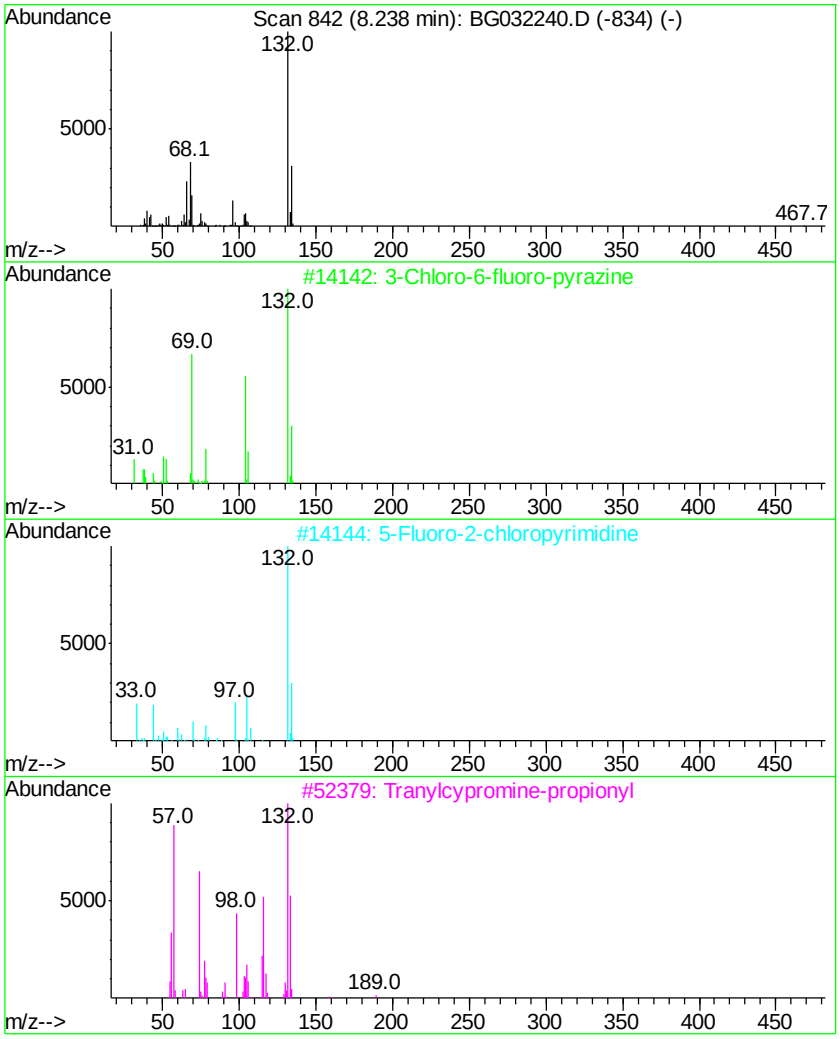
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

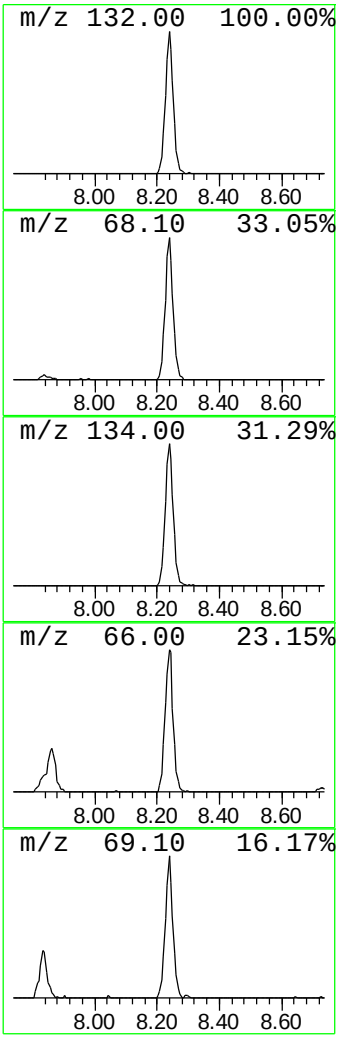
****

Peak Number 3 unknown8.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.24	39.23 ng	515195	1,4-Dichlorobenzene-d4	8.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10
5	5-Aminoindole	132	C8H8N2	005192-03-0	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

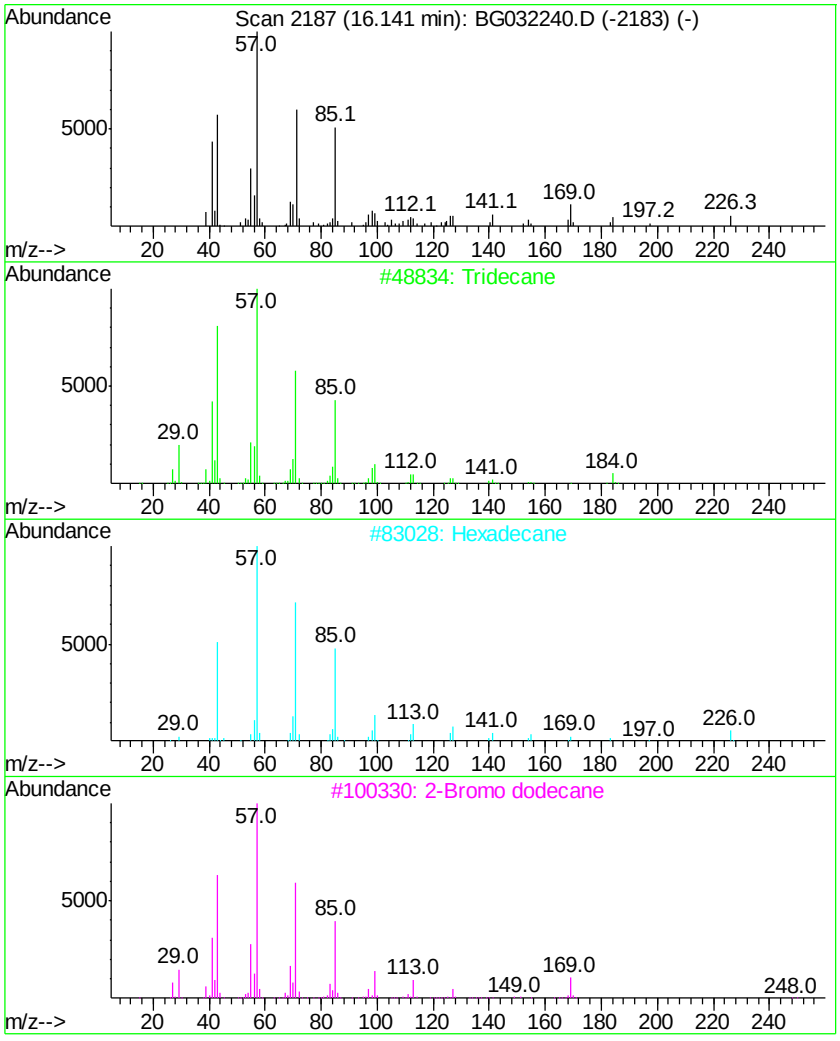
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

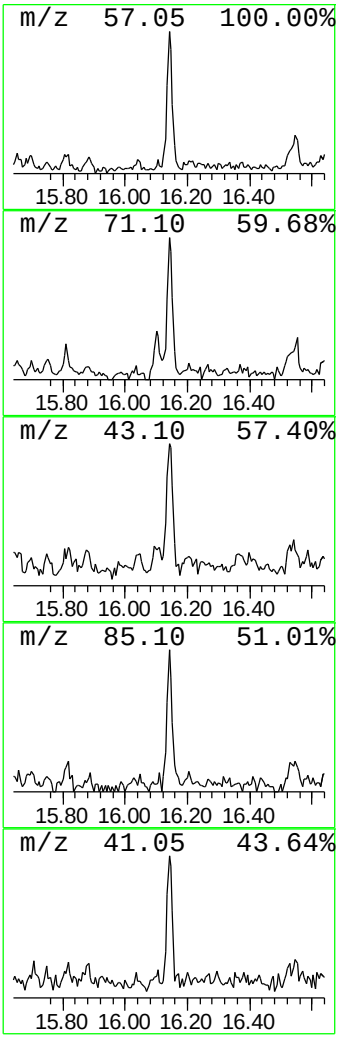
****

Peak Number 5 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	2.75 ng	80007	Acenaphthene-d10	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Hexadecane	226	C16H34	000544-76-3	87
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	74
5	Pentadecane	212	C15H32	000629-62-9	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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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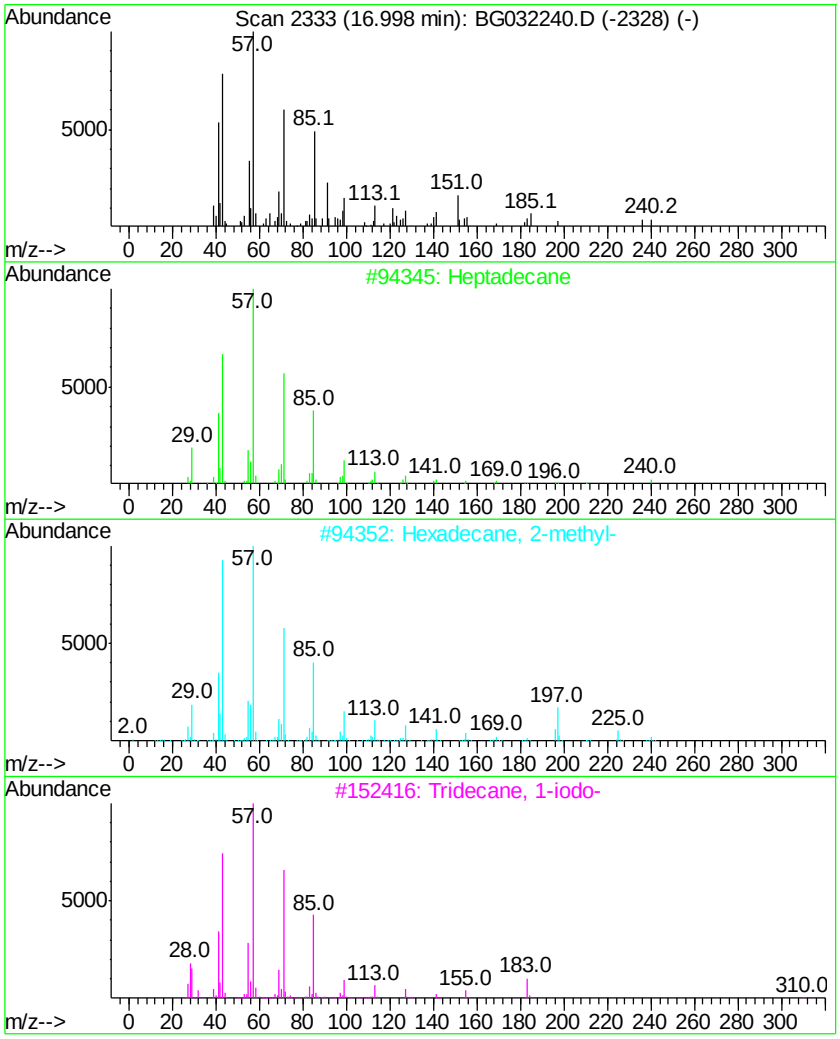
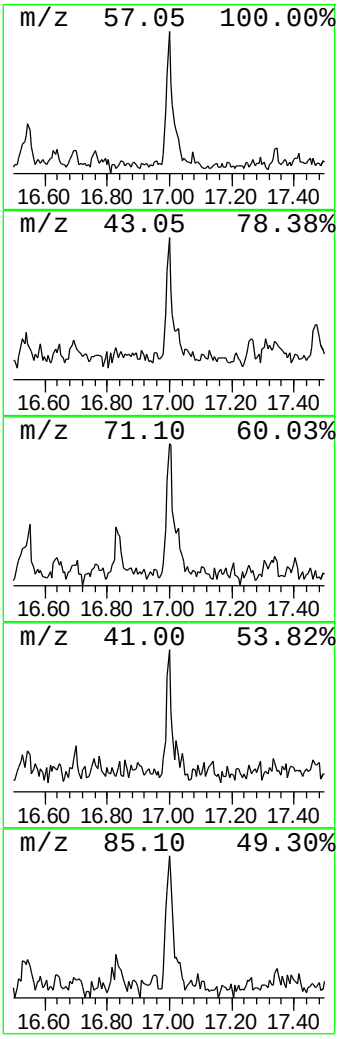
Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.00	2.94 ng	108377	Phenanthrene-d10	18.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	74
2	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	72
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	68
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	68
5	Hexacosane	366	C26H54	000630-01-3	68





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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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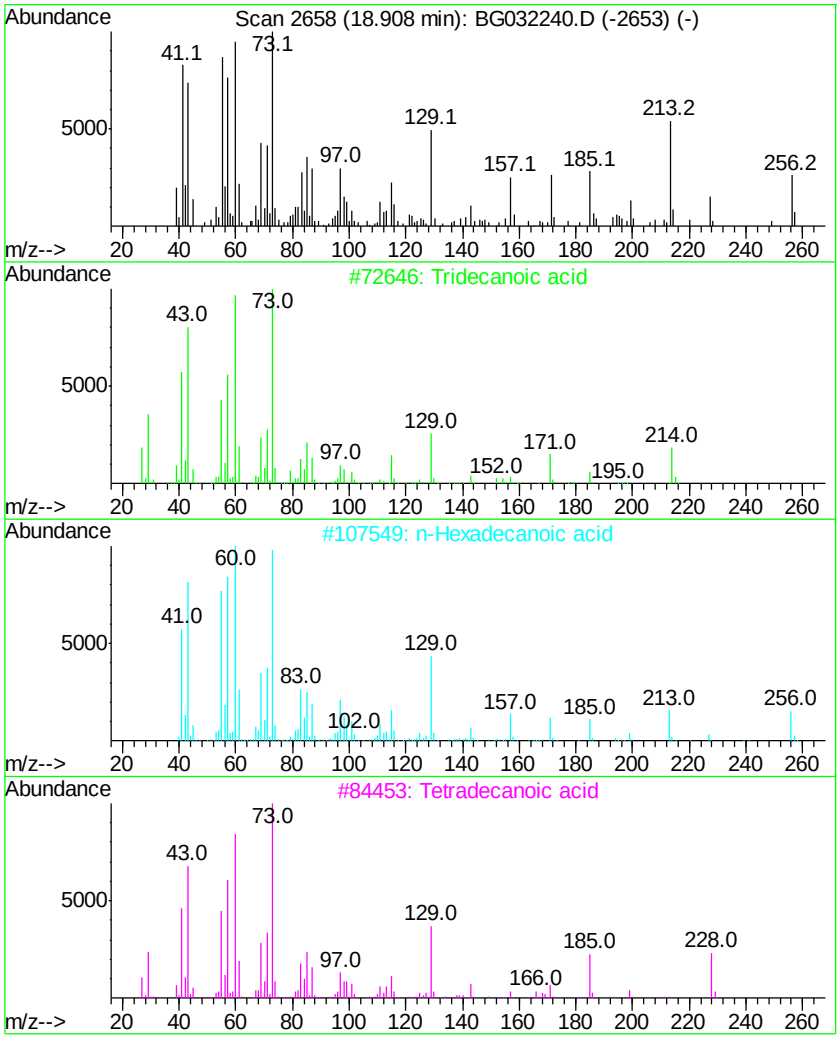
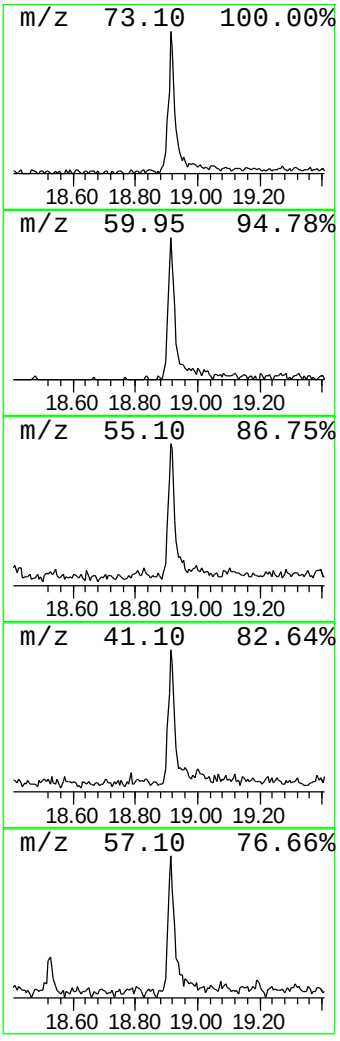
Peak Number 7 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.91	5.81 ng	214390	Phenanthrene-d10	18.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	78
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	Dodecanoic acid	200	C12H24O2	000143-07-7	45
5	n-Decanoic acid	172	C10H20O2	000334-48-5	42





Data Path : Z:\HPCHEM1\BNA G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

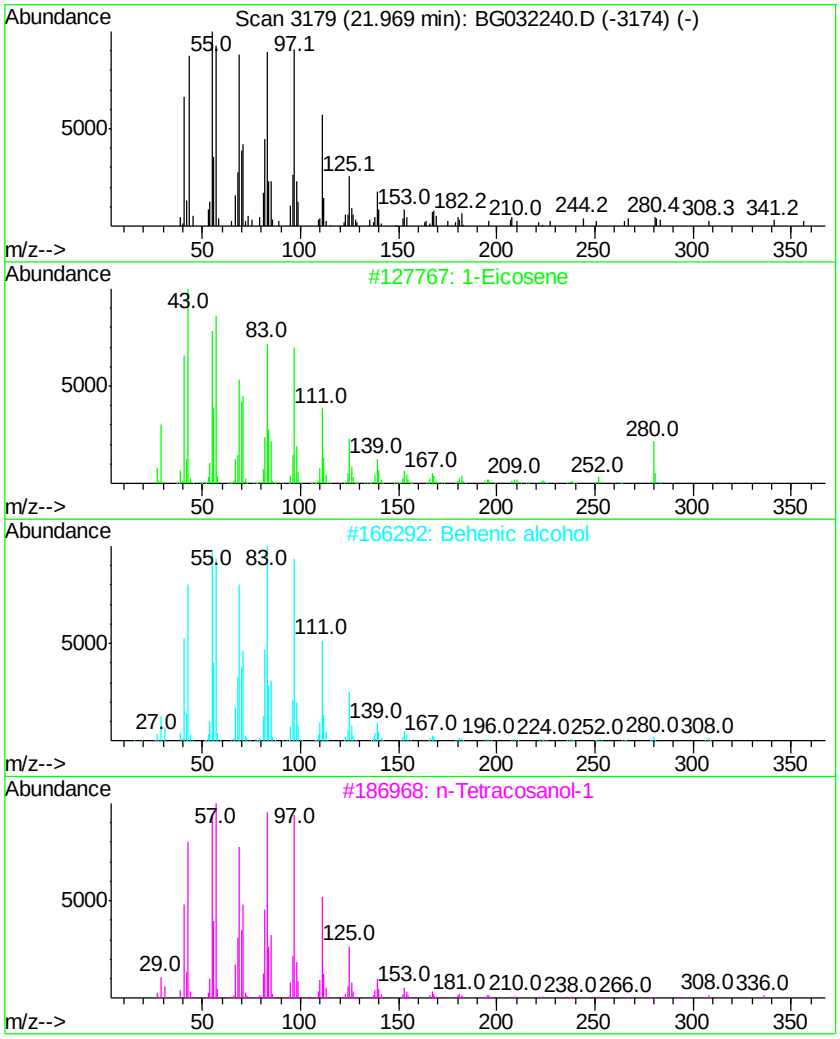
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

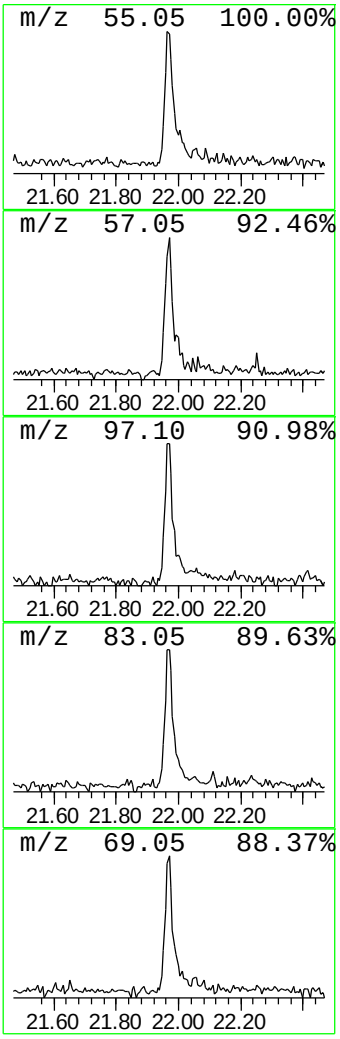
****

Peak Number 8 1-Eicosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.97	3.73 ng	182210	Chrysene-d12	22.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	97
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Docosene	308	C22H44	001599-67-3	93
5	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012318\
Data File : BG032240.D
Acq On : 23 Jan 2018 20:25
Operator : SJ/JU
Sample : J1240-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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
unknown3.39	3.39	3.3	ng	43257	1	8.73	262687	20.0
Butane, 2-methoxy...	3.47	56.2	ng	738700	1	8.73	262687	20.0
unknown8.24	8.24	39.2	ng	515195	1	8.73	262687	20.0
Tridecane	16.14	2.8	ng	80007	3	15.36	581270	20.0
Heptadecane	17.00	2.9	ng	108377	4	18.09	738000	20.0
Tridecanoic acid	18.91	5.8	ng	214390	4	18.09	738000	20.0
1-Eicosene	21.97	3.7	ng	182210	5	22.43	977764	20.0