LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112618\
Data File : BG038144.D
Acq On : 26 Nov 2018 20:43
Operator : JU/SJ
Sample : J6032-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MMTW-01

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-BG111318.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	5.632	393	399	409	rVB	348557	577348	20.58%	3.847%
2	7.230	665	671	685	rVB	227243	431601	15.38%	2.876%
3	7.612	729	736	749	rVB	622299	1133518	40.40%	7.554%
4	8.088	810	817	824	rBV	162105	273941	9.76%	1.826%
5	8.411	864	872	880	rBV	564717	1016403	36.23%	6.773%
6	9.263	1009	1017	1028	rBV	534781	999601	35.63%	6.661%
7	10.908	1288	1297	1304	rBV	225388	422271	15.05%	2.814%
8	10.984	1304	1310	1322	rVB	23052	42805	1.53%	0.285%
9	13.340	1701	1711	1721	rBV	1334416	2153560	76.76%	14.351%
10	14.721	1939	1946	1953	rBV2	359453	597910	21.31%	3.984%
11	16.214	2191	2200	2217	rBV	915878	1506071	53.68%	10.036%
12	16.413	2226	2234	2238	rBV	64072	108977	3.88%	0.726%
13	17.471	2407	2414	2425	rBV	432875	676089	24.10%	4.505%
14	18.323	2553	2559	2571	rBV2	58702	115860	4.13%	0.772%
15	19.104	2687	2692	2698	rVB2	16015	28251	1.01%	0.188%
16	19.592	2771	2775	2786	rBV5	40896	83928	2.99%	0.559%
17	20.074	2850	2857	2868	rVB	2037428	2805461	100.00%	18.695%
18	20.838	2980	2987	2991	rBV4	20618	39080	1.39%	0.260%
19	21.754	3136	3143	3157	rVB	407374	708054	25.24%	4.718%
20	21.901	3163	3168	3174	rVB2	26865	40615	1.45%	0.271%
21	22.518	3268	3273	3279	rVB2	39750	63540	2.26%	0.423%
22	23.229	3385	3394	3400	rBV	50687	105154	3.75%	0.701%
23	24.051	3526	3534	3542	rVB2	52973	122316	4.36%	0.815%
24	25.080	3690	3709	3722	rBV3	220093	796385	28.39%	5.307%
25	26.178	3887	3896	3907	rVB2	33151	101002	3.60%	0.673%
26	27.577	4123	4134	4142	rBV6	16505	56584	2.02%	0.377%

Sum of corrected areas: 15006325

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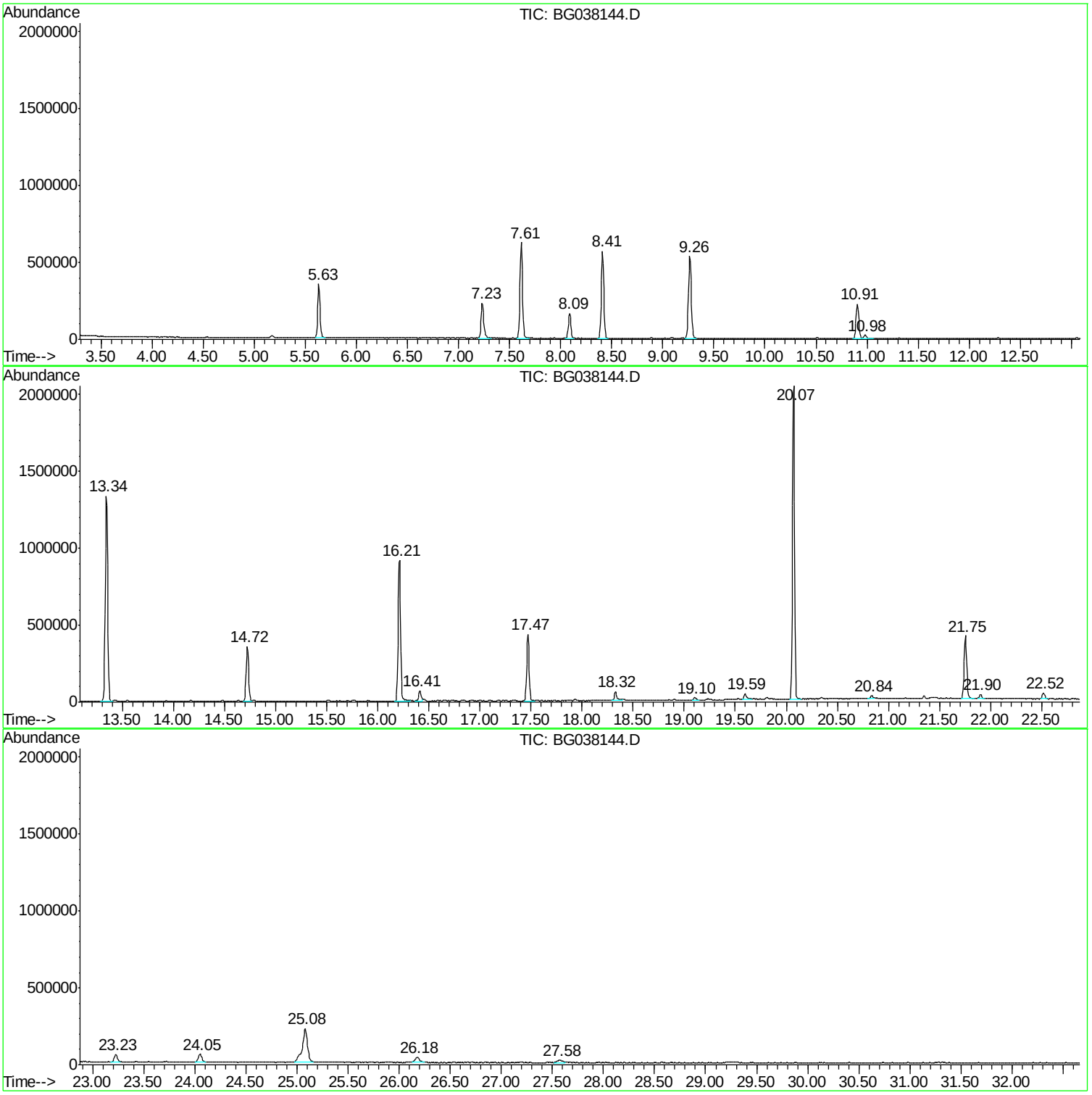
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MMTW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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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Data File : BG038144.D
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Instrument : BNA_G
ClientSampleId : MMTW-01

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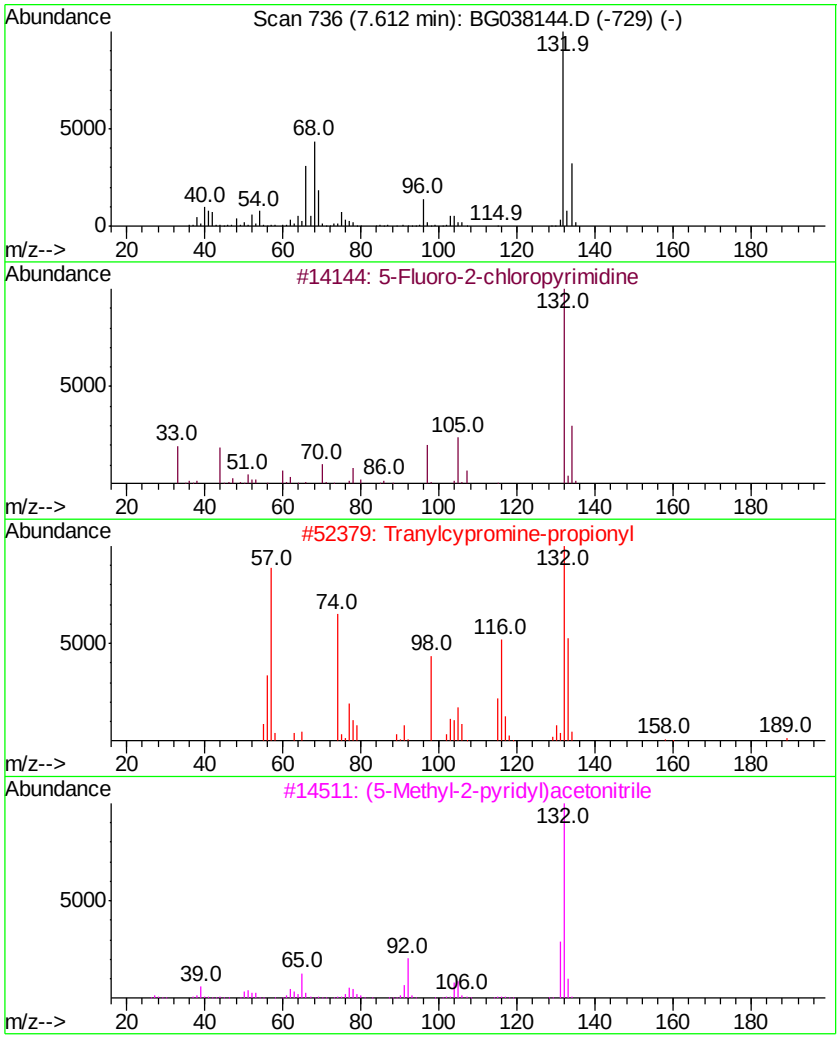
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

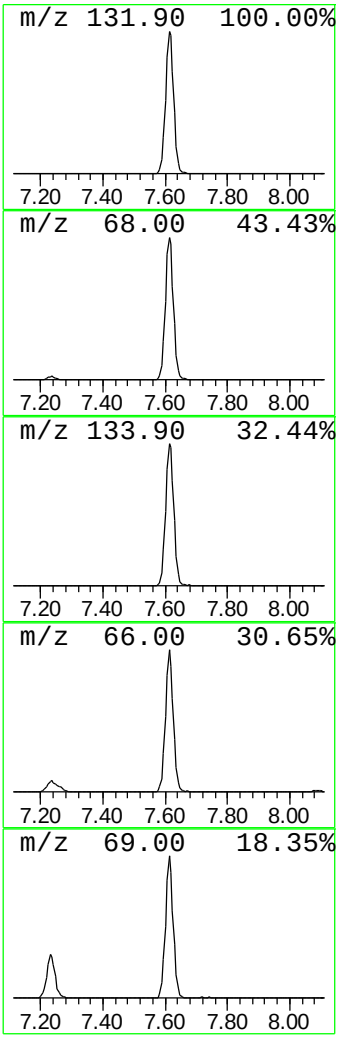
****

Peak Number 1 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	82.76 ng	1133520	1,4-Dichlorobenzene-d4	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Library Search Compound Report

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Data File : BG038144.D
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Sample : J6032-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MMTW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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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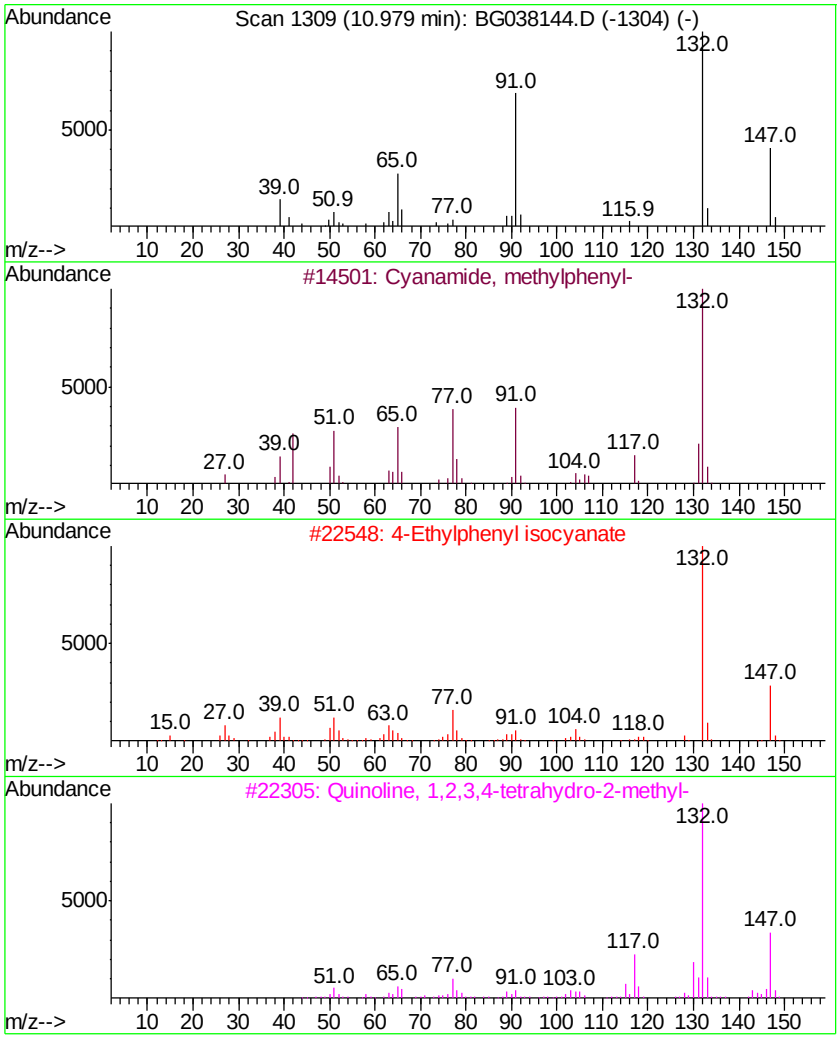
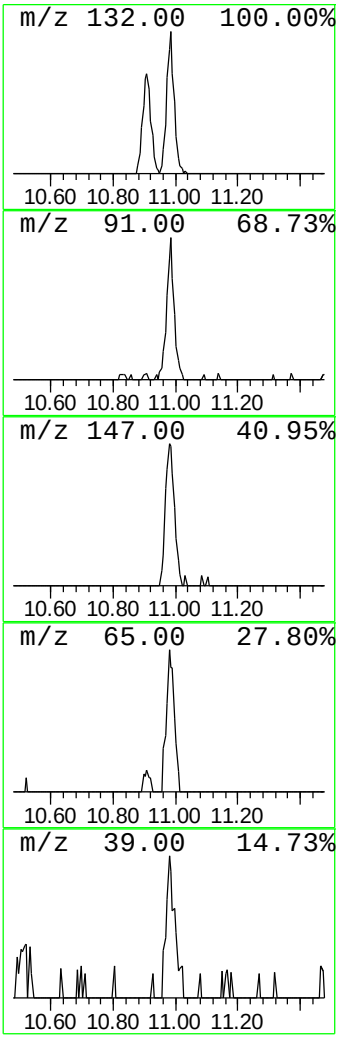
Peak Number 3 Cyanamide, methylphenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	2.03 ng	42805	Naphthalene-d8	10.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyanamide, methylphenyl-	132	C8H8N2	018773-77-8	59
2	4-Ethylphenyl isocyanate	147	C9H9NO	023138-50-3	53
3	Quinoline, 1,2,3,4-tetrahydro-2-...	147	C10H13N	001780-19-4	53
4	Benzene, (1-isocyanatoethyl)-, (S)-	147	C9H9NO	014649-03-7	53
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	47





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Acq On : 26 Nov 2018 20:43
Operator : JU/SJ
Sample : J6032-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MMTW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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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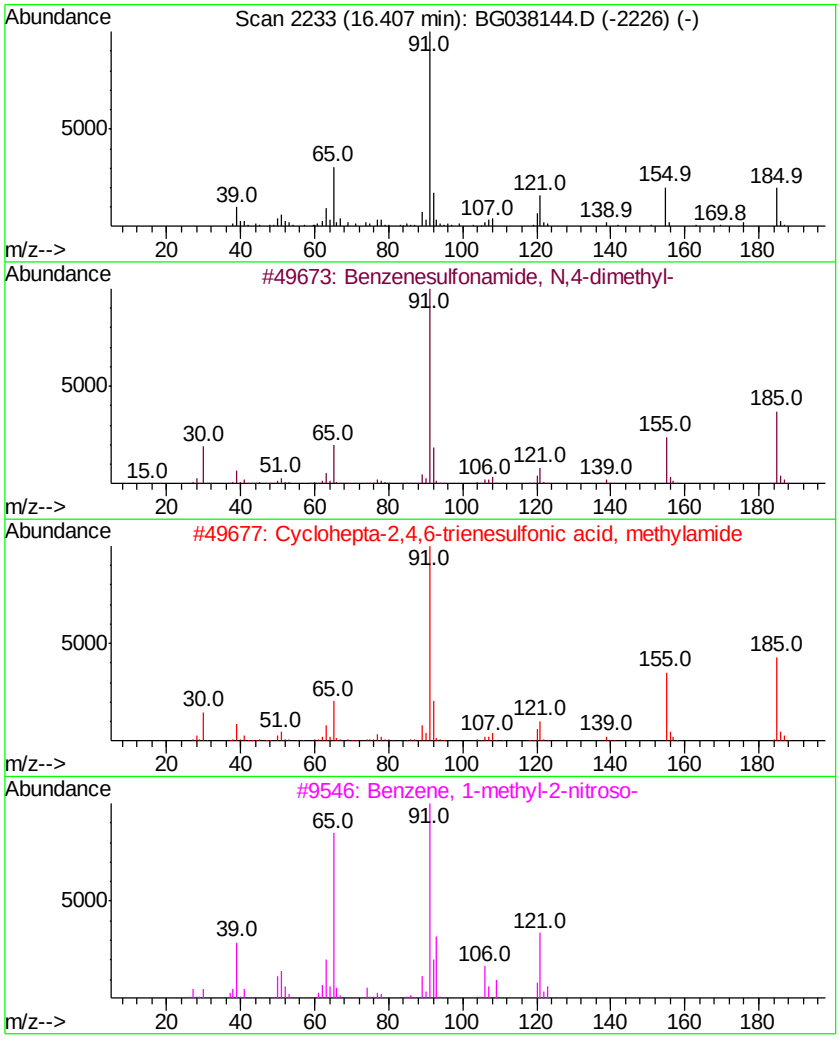
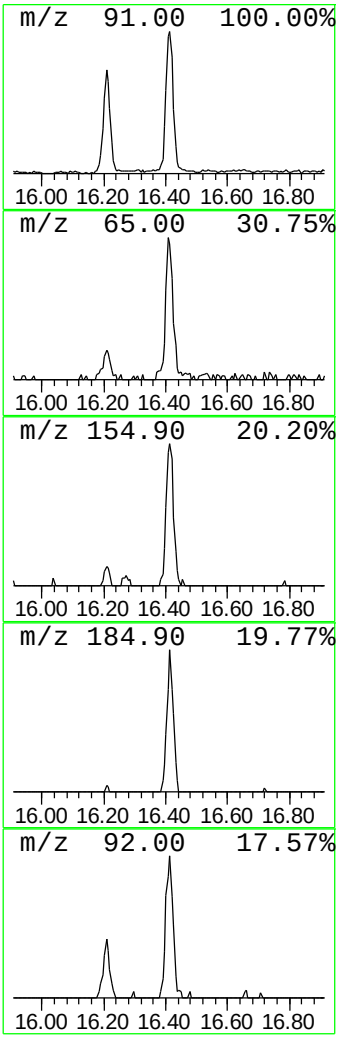
Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	3.22 ng	108977	Phenanthrene-d10	17.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	93
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	49
3	Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	49
4	Benzeneacetaldehyde	120	C8H8O	000122-78-1	45
5	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112618\
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Operator : JU/SJ
Sample : J6032-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MMTW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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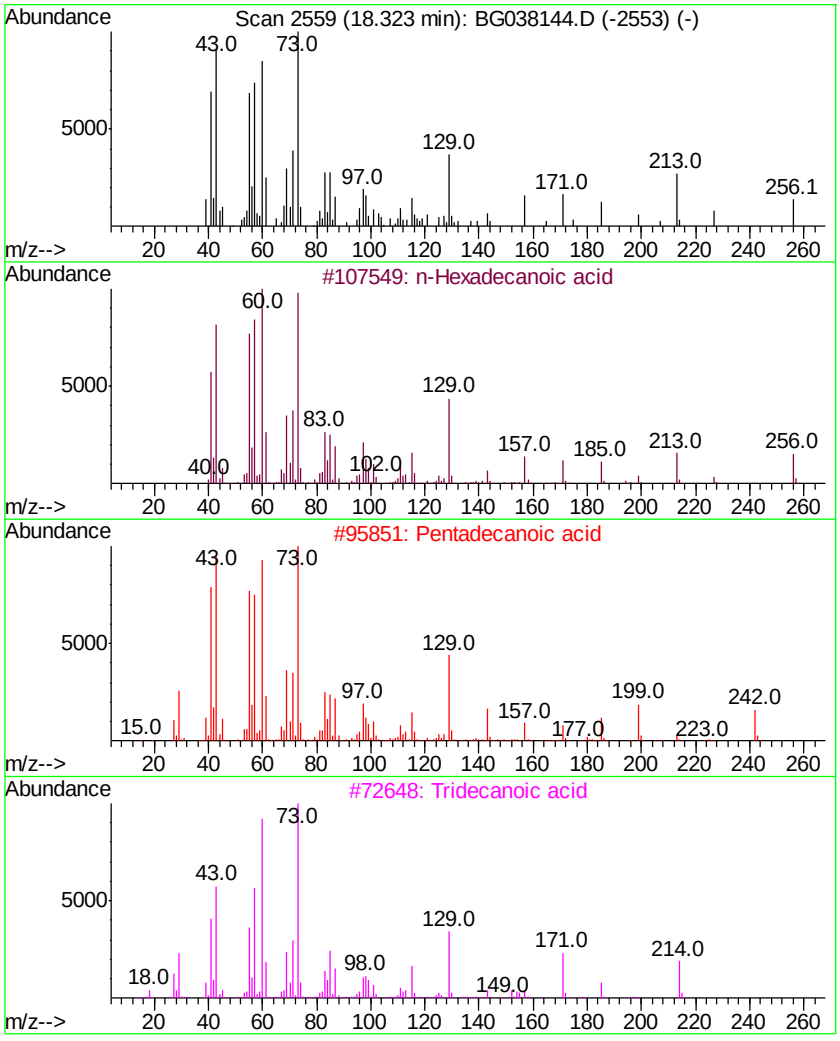
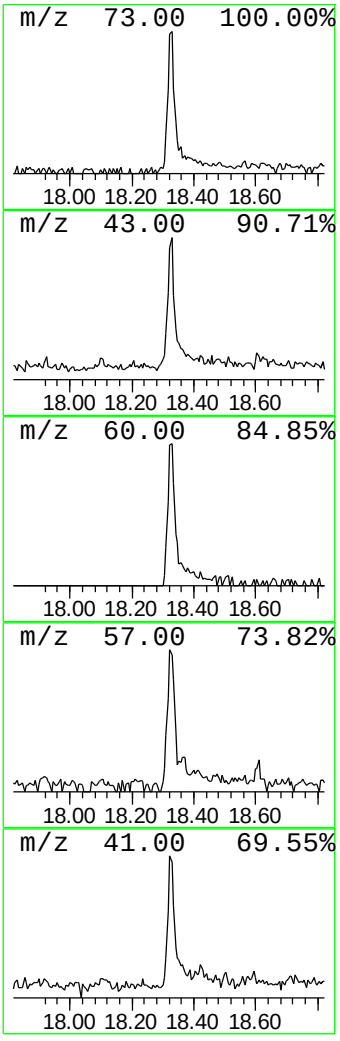
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	3.43 ng	115860	Phenanthrene-d10	17.47

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	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	52
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG112618\
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Acq On : 26 Nov 2018 20:43
Operator : JU/SJ
Sample : J6032-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MMTW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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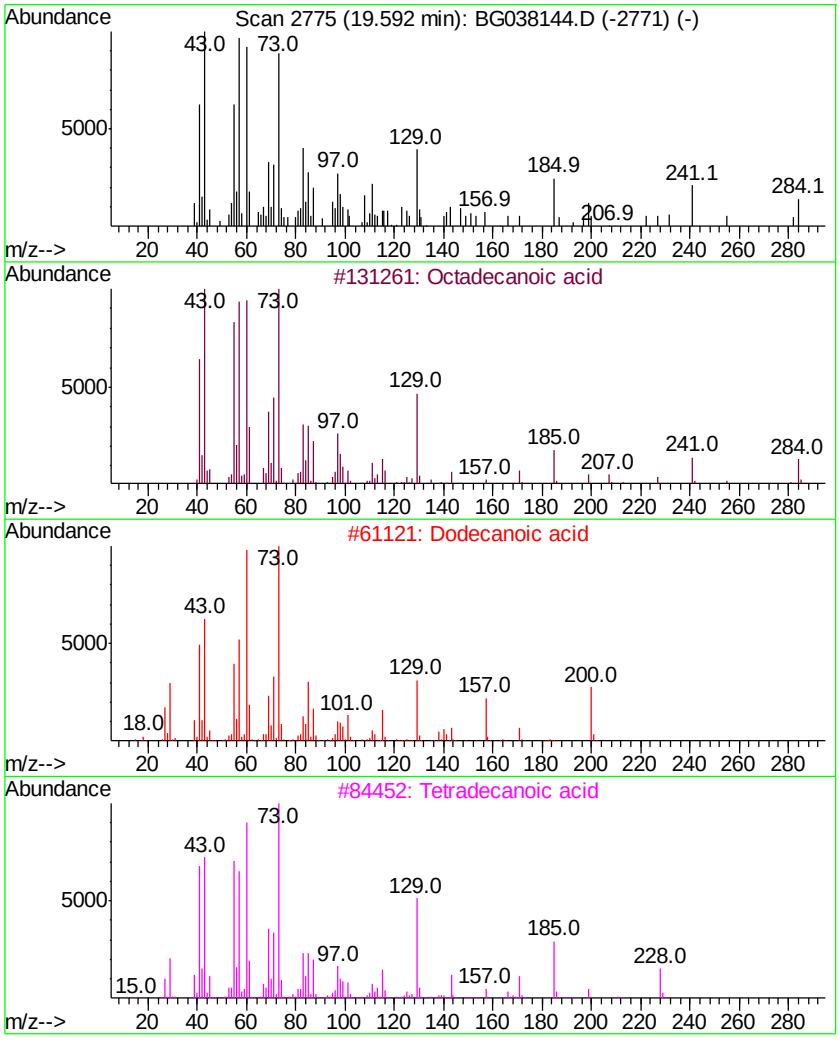
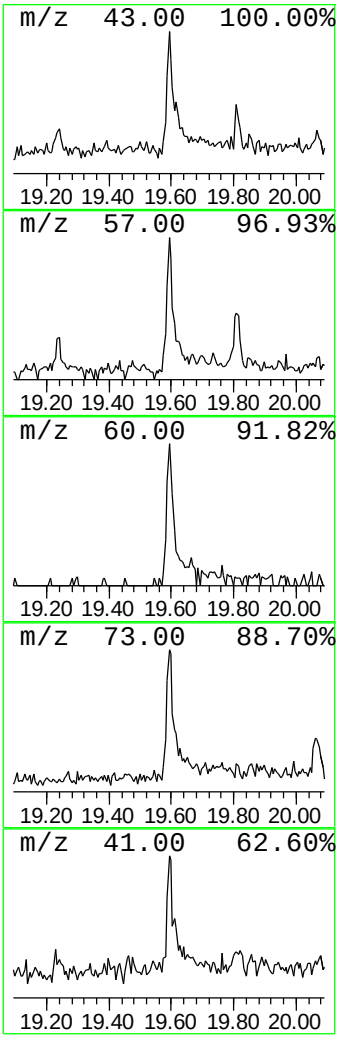
Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.59	2.48 ng	83928	Phenanthrene-d10	17.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	87
2	Dodecanoic acid	200	C12H24O2	000143-07-7	55
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4	Tridecanoic acid	214	C13H26O2	000638-53-9	49
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	43





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MMTW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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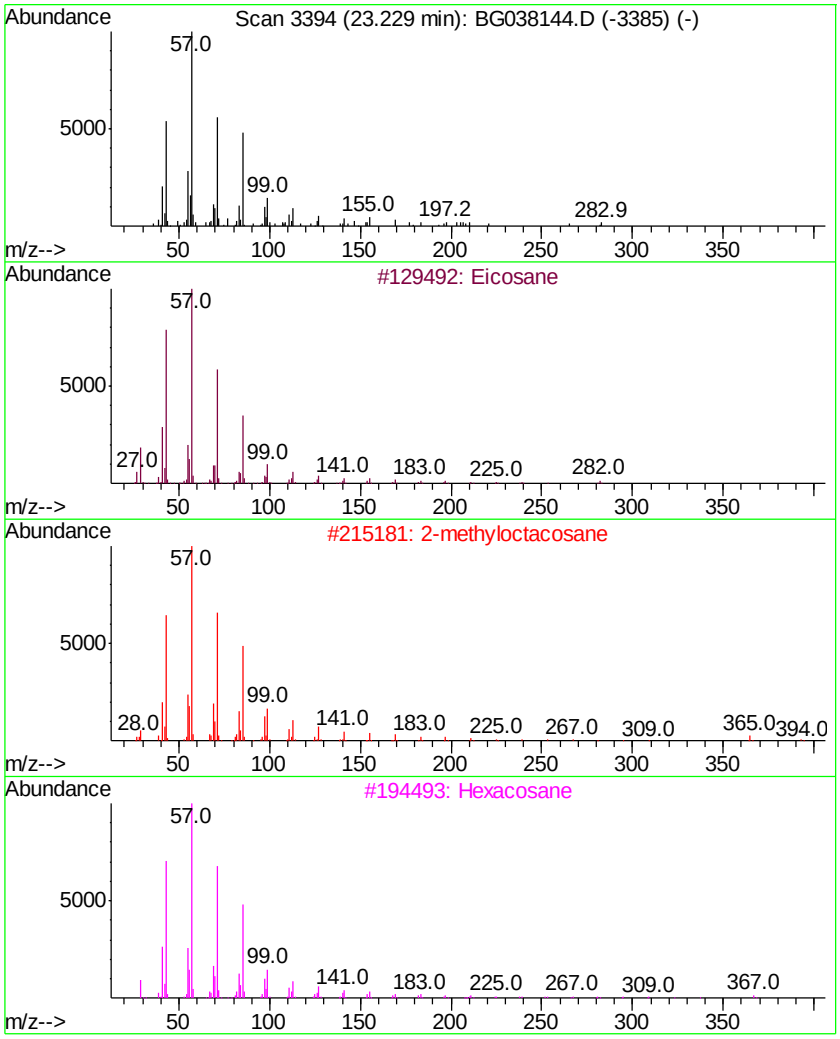
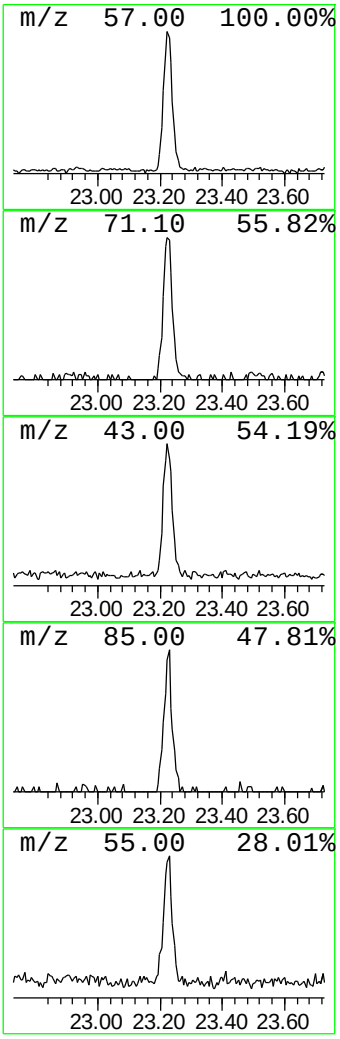
Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.23	2.97 ng	105154	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane	240	C17H36	000629-78-7	86





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Misc :
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Instrument : BNA_G
ClientSampleId : MMTW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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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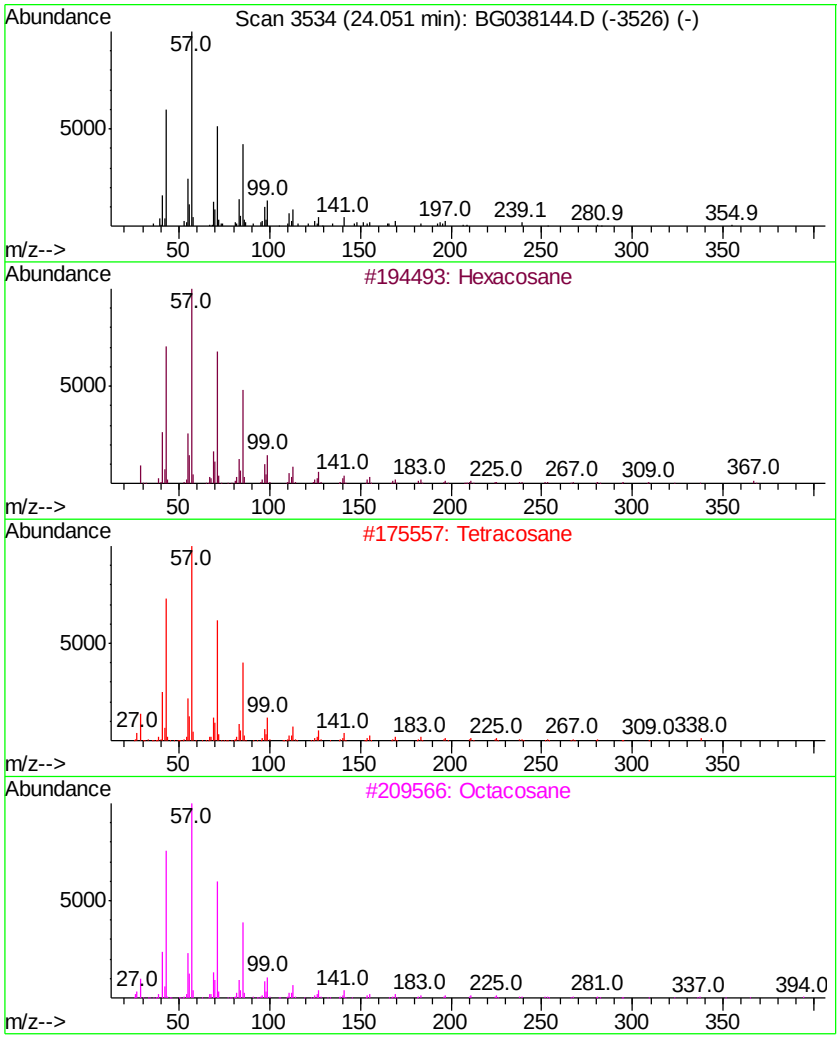
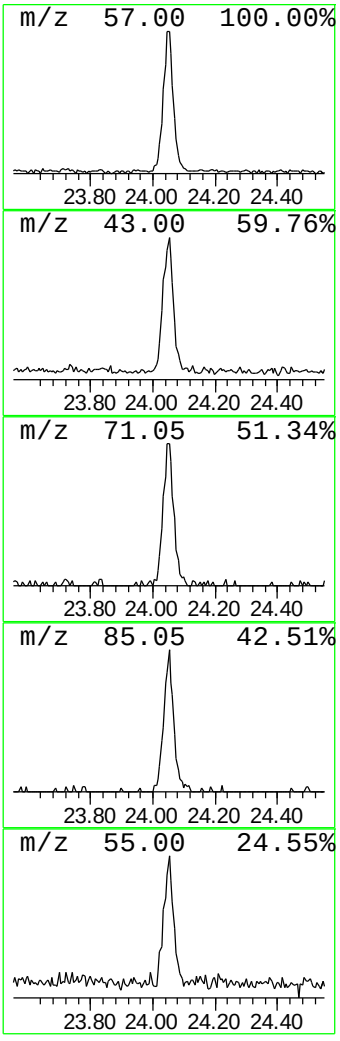
Peak Number 8 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.05	3.07 ng	122316	Perylene-d12	25.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptacosane	380	C27H56	000593-49-7	90
5	Nonadecane	268	C19H40	000629-92-5	87





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
unknown7.61	7.61	82.8	ng	1133520	1	8.09	273941	20.0
Cyanamide, methyl...	10.98	2.0	ng	42805	2	10.91	422271	20.0
Benzenesulfonamid...	16.41	3.2	ng	108977	4	17.47	676089	20.0
n-Hexadecanoic acid	18.32	3.4	ng	115860	4	17.47	676089	20.0
Octadecanoic acid	19.59	2.5	ng	83928	4	17.47	676089	20.0
Eicosane	23.23	3.0	ng	105154	5	21.75	708054	20.0
Hexacosane	24.05	3.1	ng	122316	6	25.08	796385	20.0