LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG051119\
Data File : BG040898.D
Acq On : 12 May 2019 7:51
Operator : HP/JU
Sample : K2767-18
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS012-1218-01

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-BG042319.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	3.146	5	10	18	rBV	105705	193686	4.67%	0.680%
2	3.216	18	22	36	rVB	245020	347697	8.38%	1.221%
3	5.667	430	439	449	rBV	1208821	1900454	45.82%	6.676%
4	7.276	704	713	724	rBV	1314130	2288108	55.17%	8.037%
5	7.658	770	778	790	rBV	1266971	2108843	50.85%	7.408%
6	8.134	850	859	868	rBV	212142	361939	8.73%	1.271%
7	8.457	907	914	923	rVB	804203	1373096	33.11%	4.823%
8	9.309	1051	1059	1066	rBV	789191	1399439	33.74%	4.916%
9	10.954	1332	1339	1346	rBV	282467	503114	12.13%	1.767%
10	13.387	1745	1753	1760	rBV	1792878	2731849	65.87%	9.596%
11	13.622	1784	1793	1800	rVB2	59537	98850	2.38%	0.347%
12	14.204	1886	1892	1899	rBV	346884	493269	11.89%	1.733%
13	14.762	1979	1987	1997	rBV2	496889	795970	19.19%	2.796%
14	16.248	2233	2240	2247	rBV	1921824	2844344	68.58%	9.991%
15	17.506	2448	2454	2459	rBV2	687378	1068163	25.76%	3.752%
16	17.547	2459	2461	2468	rVB2	50528	68168	1.64%	0.239%
17	18.363	2592	2600	2607	rBV2	470283	666392	16.07%	2.341%
18	18.428	2609	2611	2620	rVB3	33926	61744	1.49%	0.217%
19	18.563	2629	2634	2638	rBV3	29528	50538	1.22%	0.178%
20	18.916	2689	2694	2705	rVB7	23157	47024	1.13%	0.165%
21	19.215	2740	2745	2751	rBV7	28150	62498	1.51%	0.220%
22	19.274	2752	2755	2762	rVB6	35152	61401	1.48%	0.216%
23	19.550	2797	2802	2807	rVB	107478	160548	3.87%	0.564%
24	19.627	2808	2815	2822	rBV2	107384	175530	4.23%	0.617%
25	19.909	2859	2863	2870	rVB	167334	242477	5.85%	0.852%
26	20.103	2890	2896	2907	rVB	3238712	4147272	100.00%	14.568%
27	20.373	2936	2942	2945	rBV7	34272	74415	1.79%	0.261%
28	20.696	2993	2997	3000	rBV2	34901	52570	1.27%	0.185%
29	20.743	3002	3005	3014	rVB4	29210	47448	1.14%	0.167%
30	21.383	3110	3114	3122	rBV2	300258	530152	12.78%	1.862%
31	21.789	3174	3183	3188	rBV2	721455	1328420	32.03%	4.666%
32	21.836	3188	3191	3200	rVB	74075	117724	2.84%	0.414%
33	22.617	3319	3324	3331	rVB10	29004	72065	1.74%	0.253%
34	23.275	3431	3436	3451	rVB5	53489	129213	3.12%	0.454%

LSC Area Percent Report

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Acq On : 12 May 2019 7:51
Operator : HP/JU
Sample : K2767-18
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : P026-SS012-1218-01

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-BG042319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.475	3464	3470	3477	rVB2	128099	264215	6.37%	0.928%
36	24.057	3562	3569	3573	rBV5	35305	94167	2.27%	0.331%
37	24.809	3692	3697	3705	rVB2	32276	84187	2.03%	0.296%
38	24.962	3718	3723	3733	rVB3	43371	122563	2.96%	0.431%
39	25.138	3739	3753	3764	rBV2	419363	1239639	29.89%	4.354%
40	26.430	3966	3973	3976	rBV8	27009	59224	1.43%	0.208%

Sum of corrected areas: 28468415

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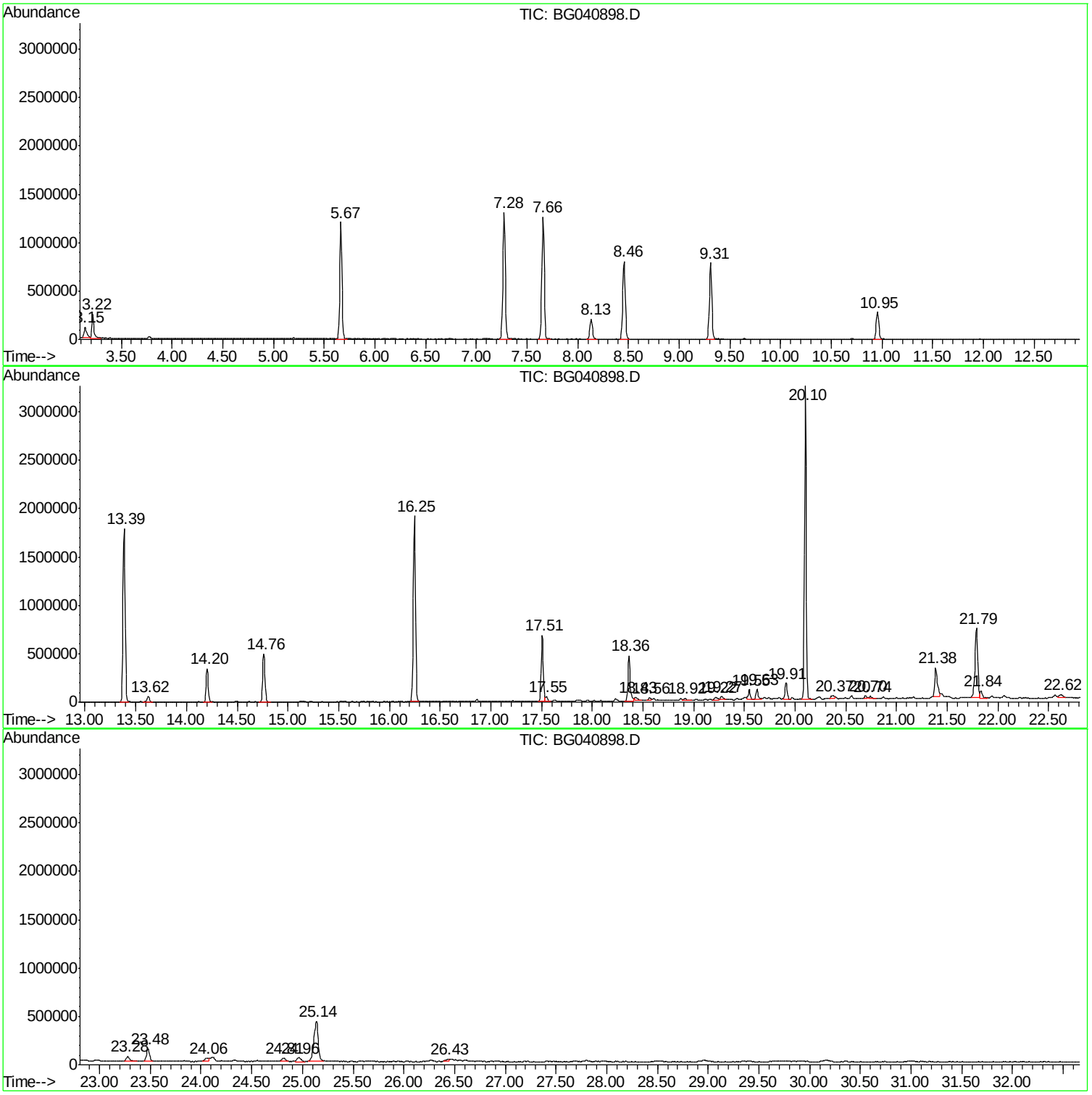
BNA_G
ClientSampleId :
P026-SS012-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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Instrument : BNA_G
ClientSampleId : P026-SS012-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

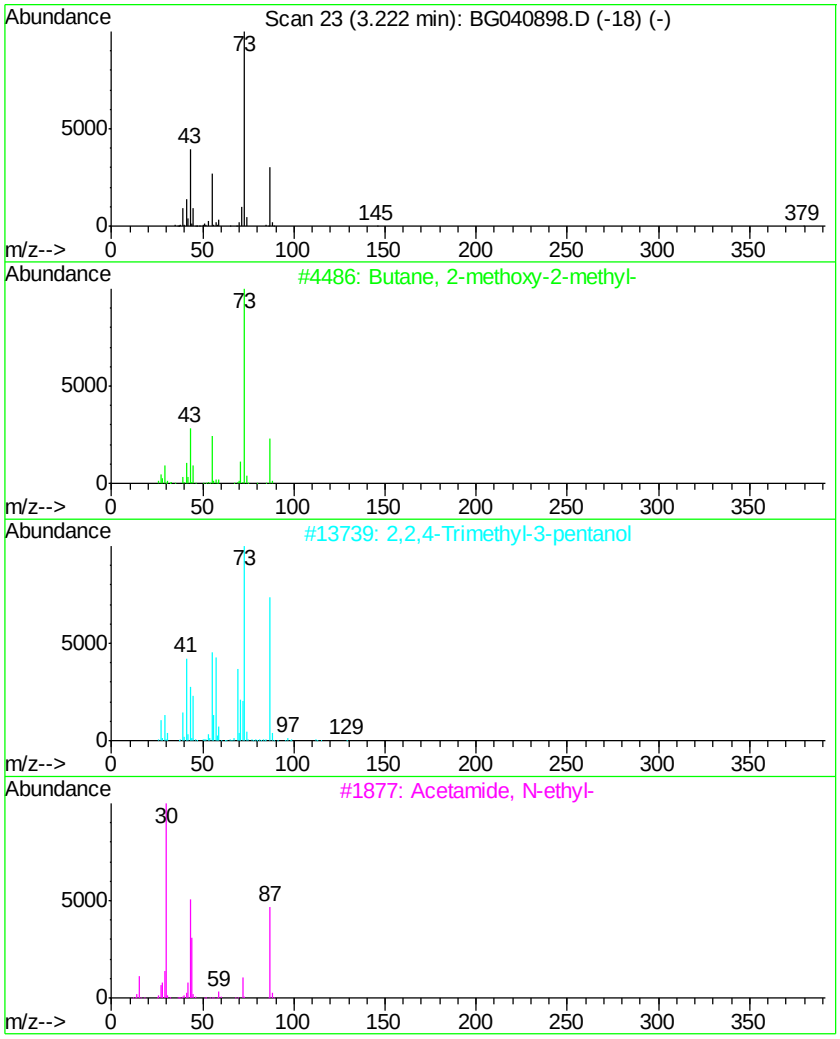
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

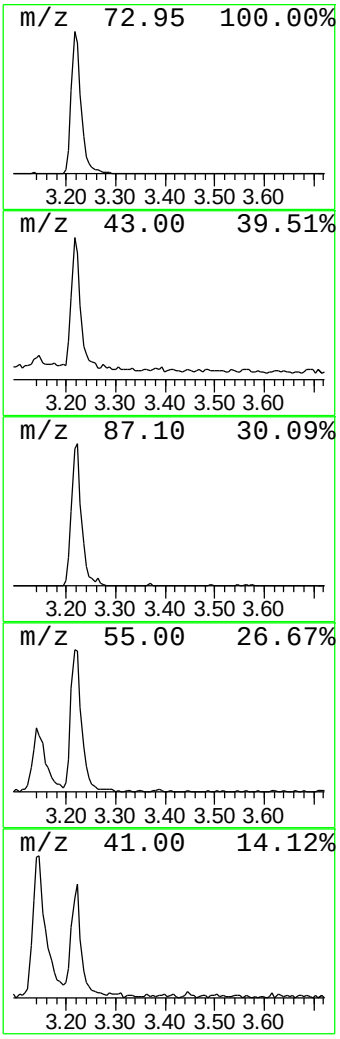
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	19.21 ng	347697	1,4-Dichlorobenzene-d4	8.13

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	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : P026-SS012-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

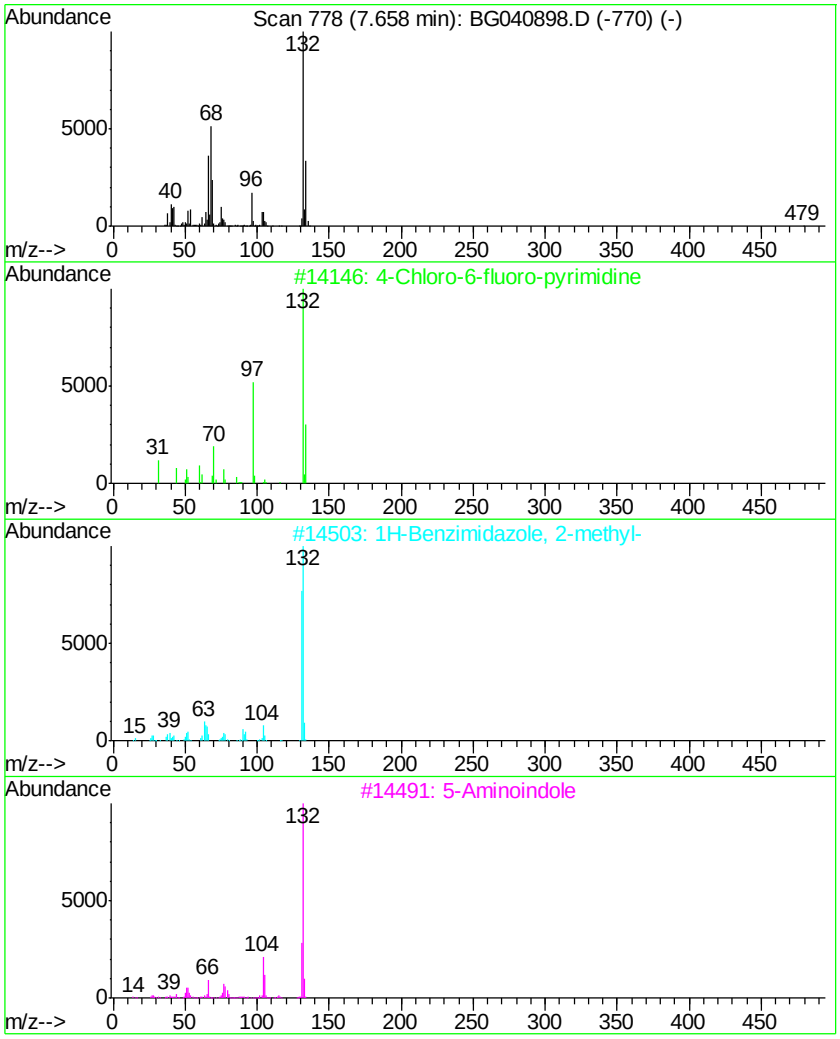
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

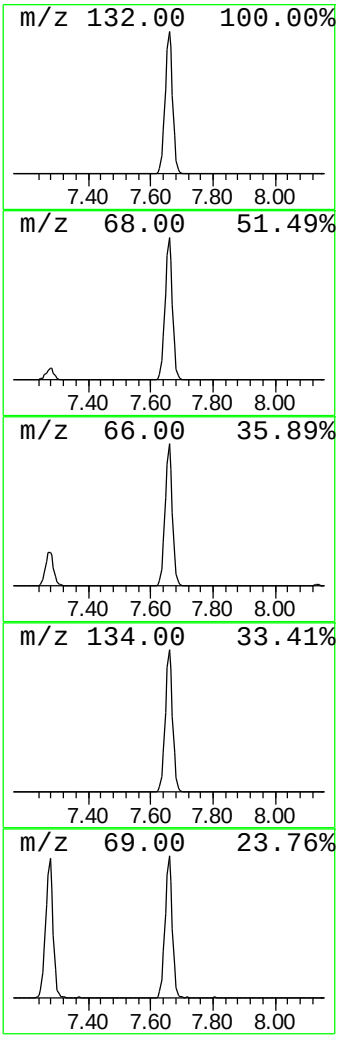
****

Peak Number 3 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	116.53 ng	2108840	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14





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Misc :
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Instrument : BNA_G
ClientSampleId : P026-SS012-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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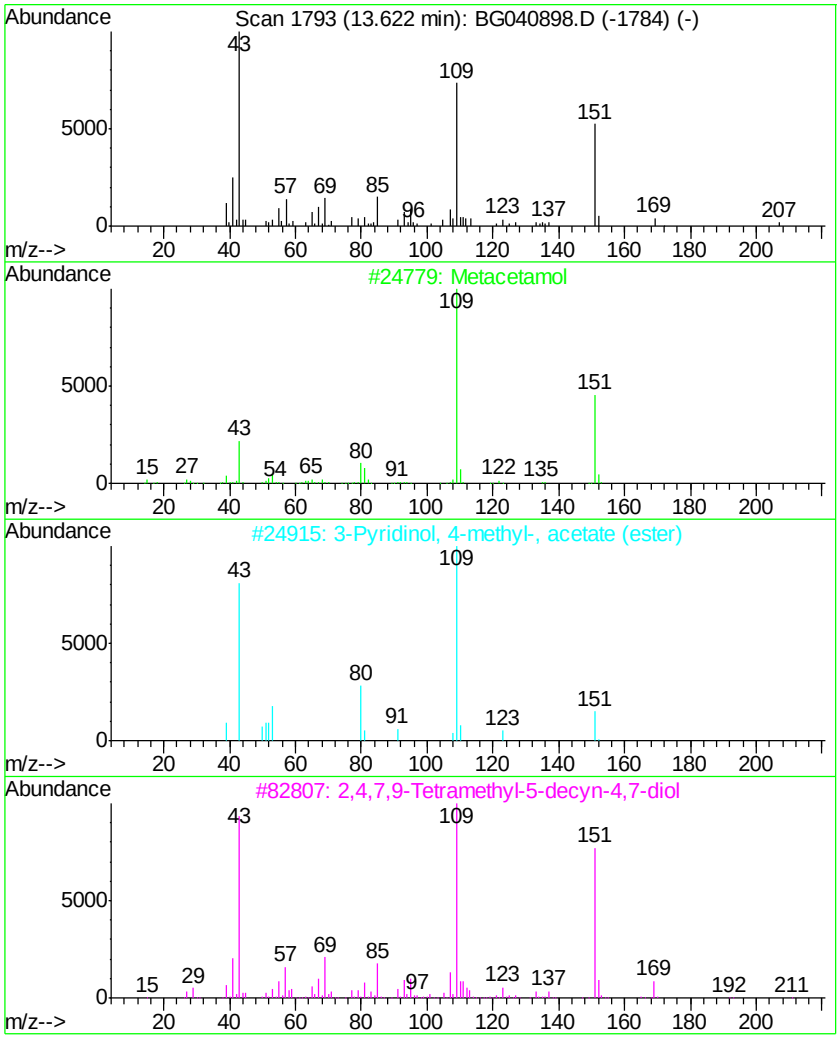
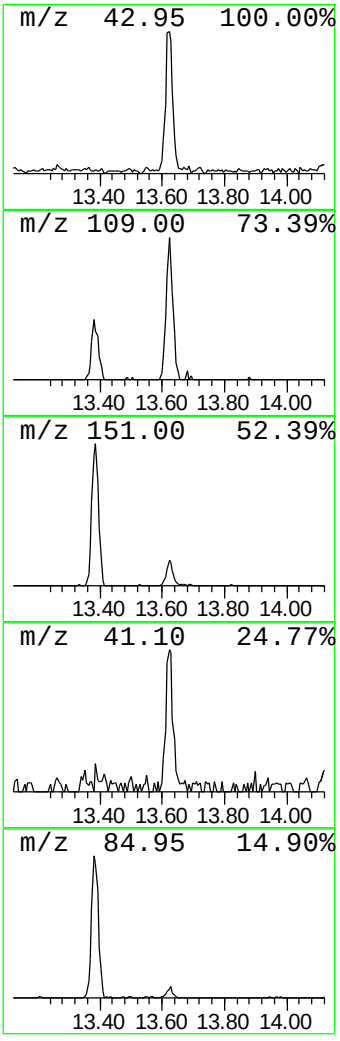
Peak Number 5 Metacetamol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	2.48 ng	98850	Acenaphthene-d10	14.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Metacetamol	151	C8H9NO2	000621-42-1	64
2	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	64
3	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	58
4	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	45
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	45





Library Search Compound Report

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Operator : HP/JU
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Instrument : BNA_G
ClientSampleId : P026-SS012-1218-01

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TIC Library : C:\Database\NIST11.L
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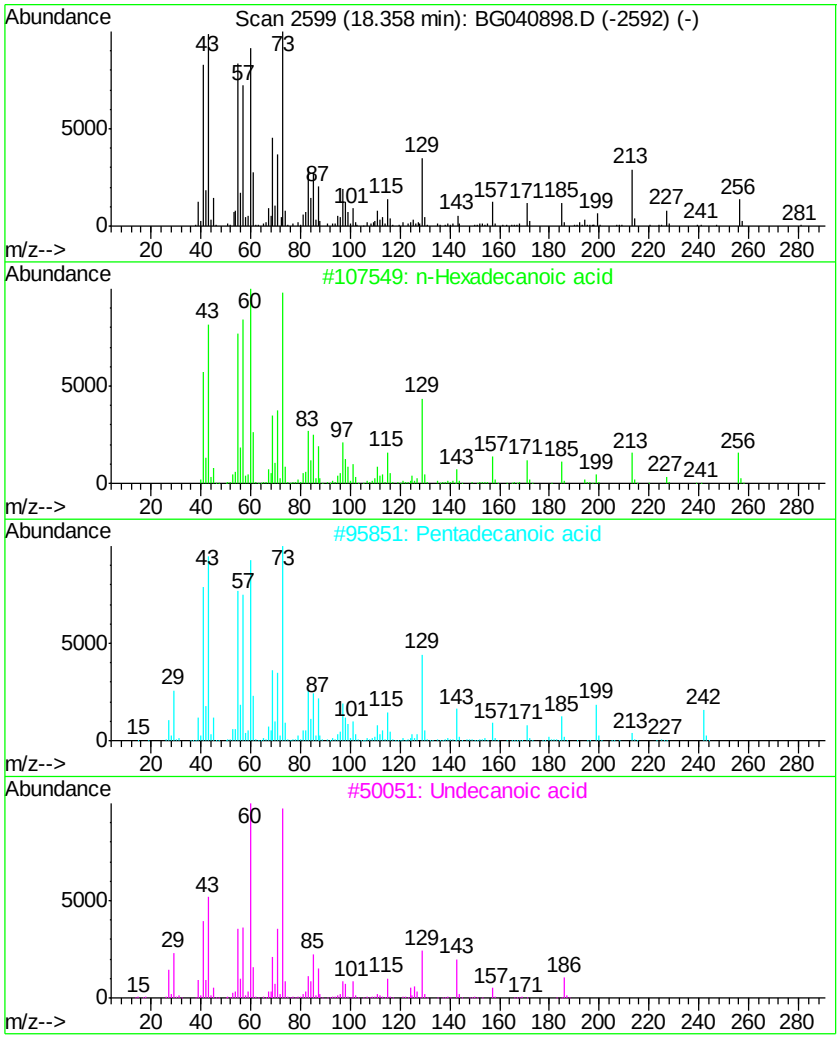
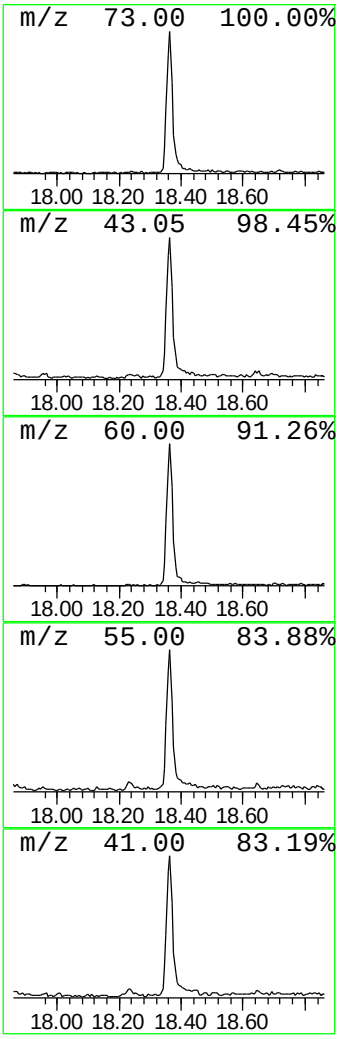
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	12.48 ng	666392	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Misc :
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Instrument : BNA_G
ClientSampleId : P026-SS012-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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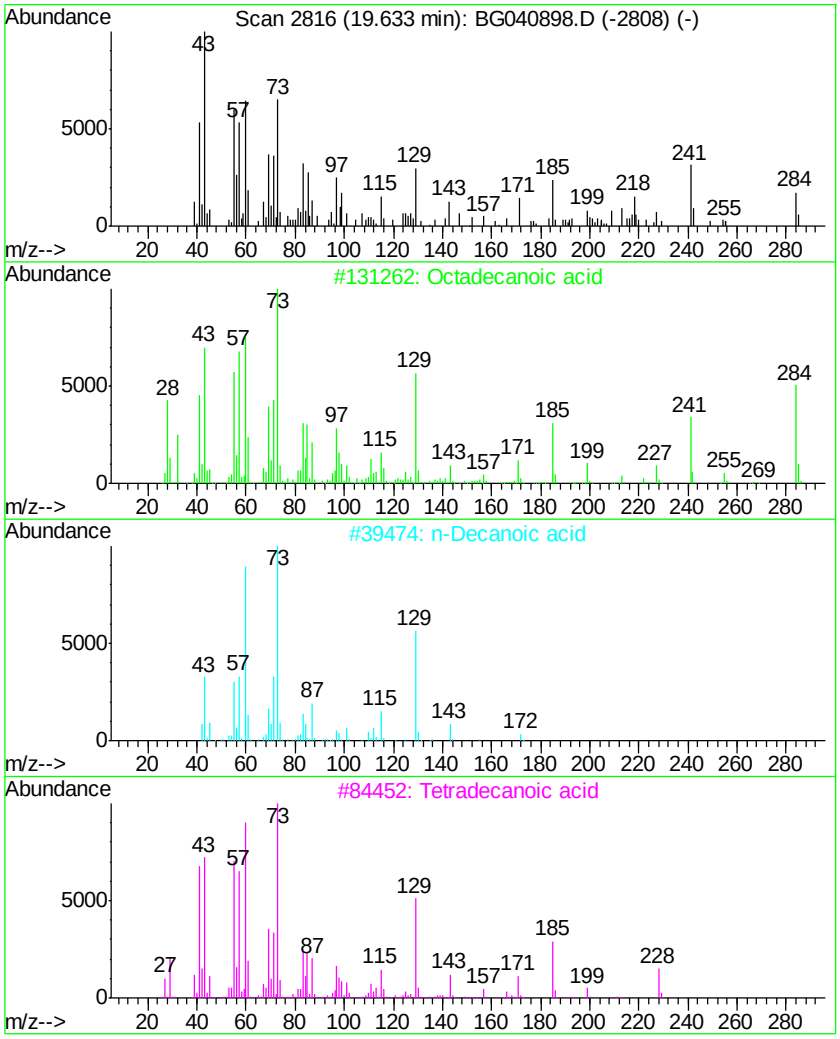
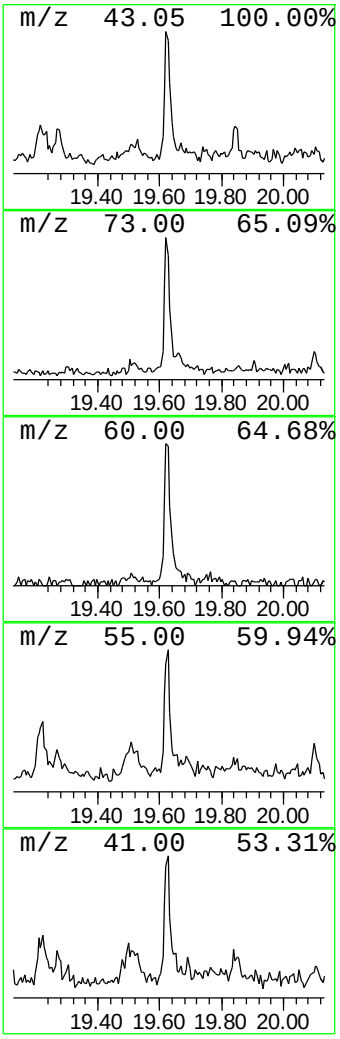
Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.63	3.29 ng	175530	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	53
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46





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Instrument : BNA_G
ClientSampleId : P026-SS012-1218-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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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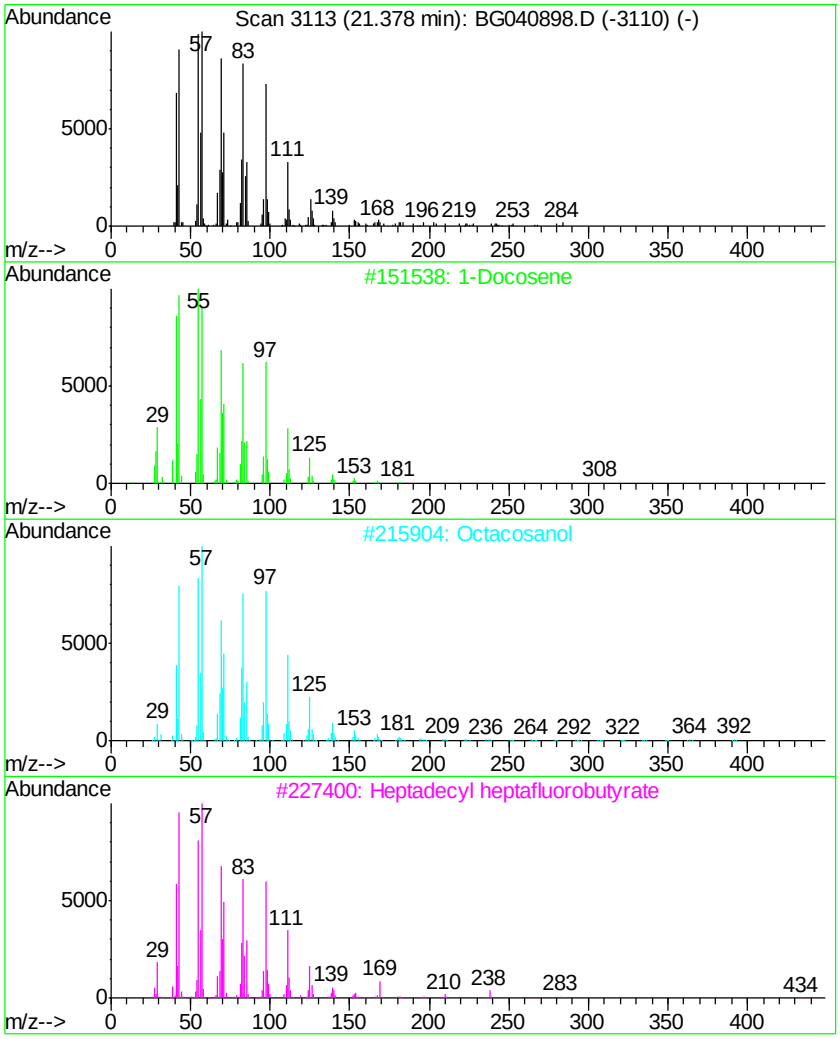
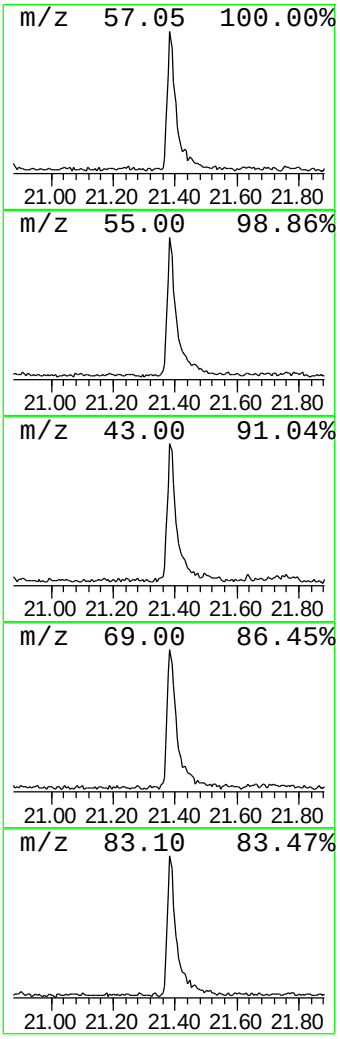
Peak Number 8 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	7.98 ng	530152	Chrysene-d12	21.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Octacosanol	410	C28H58O	000557-61-9	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

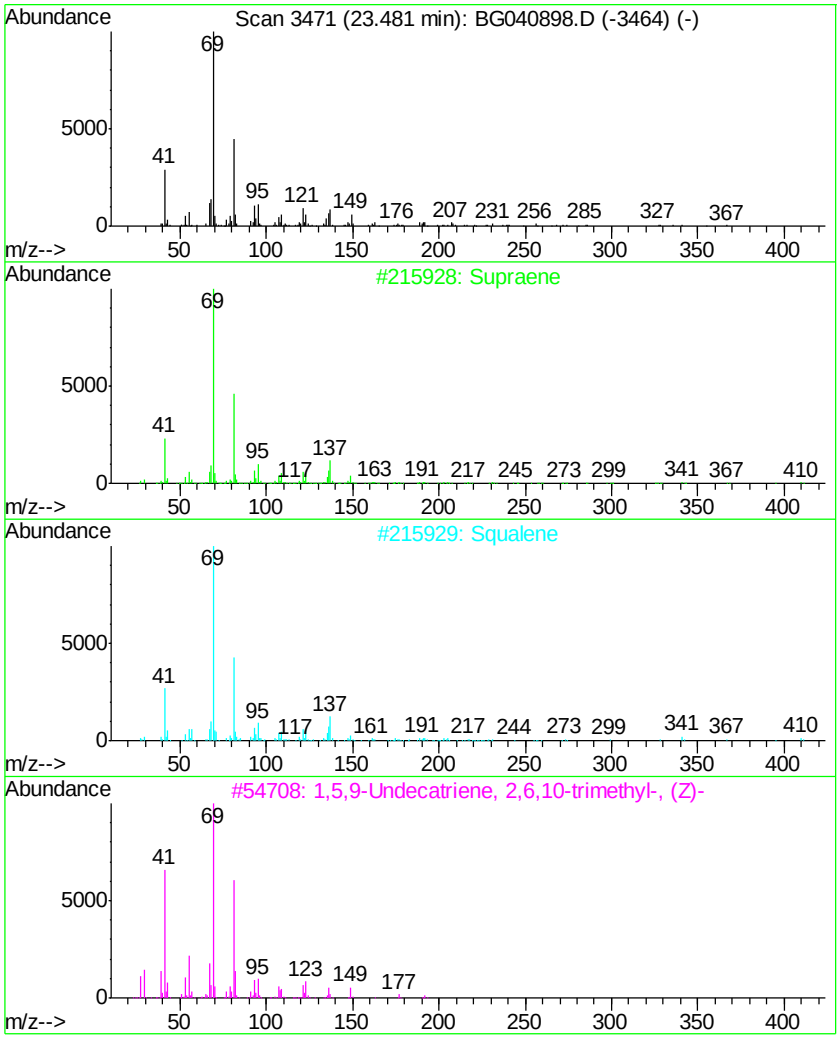
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

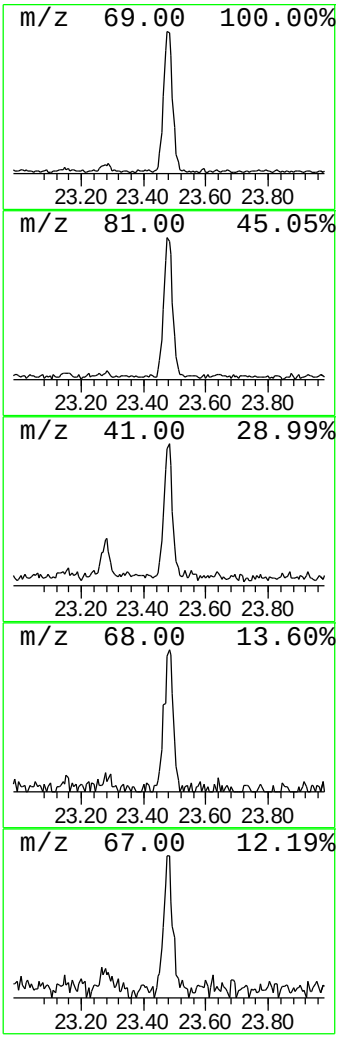
****

Peak Number 9 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.48	4.26 ng	264215	Perylene-d12	25.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	Squalene	410	C30H50	000111-02-4	83
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG042319.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...	3.22	19.2	ng	347697	1	8.13	361939	20.0
unknown7.66	7.66	116.5	ng	2108840	1	8.13	361939	20.0
Metacetamol	13.62	2.5	ng	98850	3	14.76	795970	20.0
n-Hexadecanoic acid	18.36	12.5	ng	666392	4	17.51	1068160	20.0
Octadecanoic acid	19.63	3.3	ng	175530	4	17.51	1068160	20.0
1-Docosene	21.38	8.0	ng	530152	5	21.79	1328420	20.0
Supraene	23.48	4.3	ng	264215	6	25.14	1239640	20.0