LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110618\
Data File : BG037846.D
Acq On : 6 Nov 2018 20:02
Operator : JU/SJ
Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

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-BG101818.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	5.182	315	322	329	rVB2	16952	30622	1.08%	0.165%
2	5.635	392	399	412	rBV	353756	594682	20.94%	3.200%
3	7.239	664	672	684	rBV2	236626	486368	17.12%	2.617%
4	7.621	729	737	750	rBV	670645	1189427	41.88%	6.400%
5	8.096	811	818	825	rBV	184656	325092	11.45%	1.749%
6	8.420	863	873	882	rBV	609870	1114189	39.23%	5.995%
7	9.272	1007	1018	1028	rBV	525441	980826	34.53%	5.278%
8	10.917	1289	1298	1307	rBV	273086	511343	18.00%	2.751%
9	11.575	1403	1410	1419	rBV	44229	85977	3.03%	0.463%
10	13.349	1703	1712	1720	rBV	1542397	2468612	86.92%	13.283%
11	13.978	1814	1819	1826	rBV	28702	43776	1.54%	0.236%
12	14.172	1846	1852	1857	rBV	50416	77423	2.73%	0.417%
13	14.730	1939	1947	1956	rBV2	454261	751272	26.45%	4.043%
14	15.523	2077	2082	2088	rVB4	35064	56810	2.00%	0.306%
15	15.934	2143	2152	2157	rBV4	18113	46211	1.63%	0.249%
16	16.216	2193	2200	2209	rBV	995835	1583183	55.74%	8.519%
17	16.410	2227	2233	2239	rBV2	95403	191354	6.74%	1.030%
18	16.998	2329	2333	2338	rBV4	47854	70894	2.50%	0.381%
19	17.239	2370	2374	2378	rBV2	46142	59569	2.10%	0.321%
20	17.474	2409	2414	2428	rVB2	502579	816049	28.73%	4.391%
21	17.844	2474	2477	2483	rBV4	25142	43675	1.54%	0.235%
22	18.332	2556	2560	2564	rBV3	63556	101832	3.59%	0.548%
23	19.136	2693	2697	2705	rVB6	70848	133364	4.70%	0.718%
24	19.536	2761	2765	2770	rBV	988105	1196839	42.14%	6.440%
25	20.077	2851	2857	2867	rVB	2091957	2840197	100.00%	15.283%
26	21.164	3037	3042	3048	rVB	168108	220771	7.77%	1.188%
27	21.610	3113	3118	3127	rVB	299687	433456	15.26%	2.332%
28	21.757	3137	3143	3155	rVB2	439625	811774	28.58%	4.368%
29	22.527	3271	3274	3281	rVB2	30074	47002	1.65%	0.253%
30	22.926	3337	3342	3347	rVB5	24783	44336	1.56%	0.239%
31	23.243	3390	3396	3408	rVB4	54196	127750	4.50%	0.687%
32	23.437	3425	3429	3435	rBV4	20647	37967	1.34%	0.204%
33	24.066	3529	3536	3544	rVB4	43972	106299	3.74%	0.572%
34	25.088	3696	3710	3739	rVB2	215859	831311	29.27%	4.473%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110618\
Data File : BG037846.D
Acq On : 6 Nov 2018 20:02
Operator : JU/SJ
Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

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-BG101818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	26.211	3892	3901	3911	rVB4	28196	89221	3.14%	0.480%
36	27.597	4129	4137	4139	rBV7	14818	34711	1.22%	0.187%

Sum of corrected areas: 18584184

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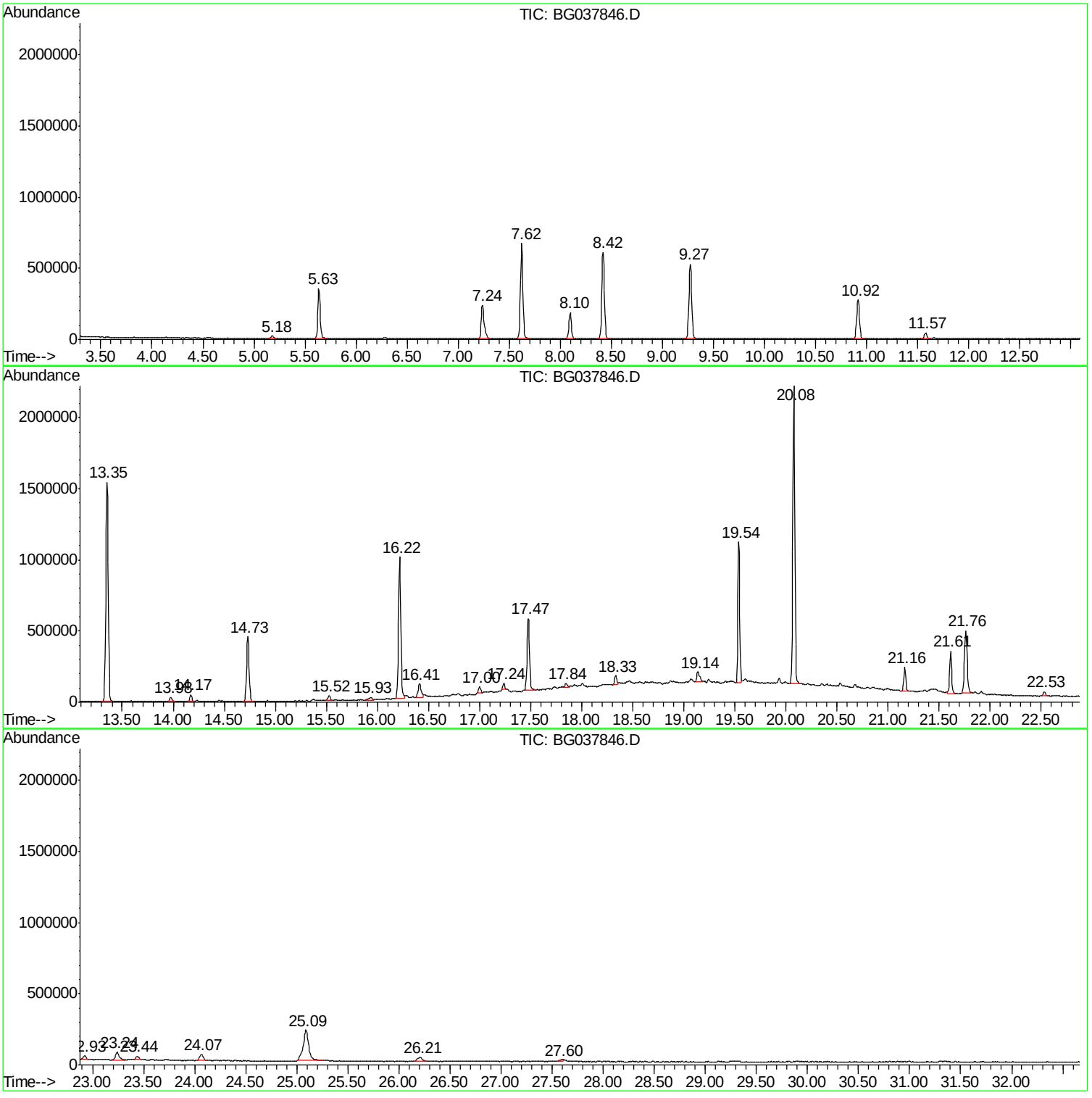
Instrument :
BNA_G
ClientSampleId :
BS-DRUM-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110618\
Data File : BG037846.D
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

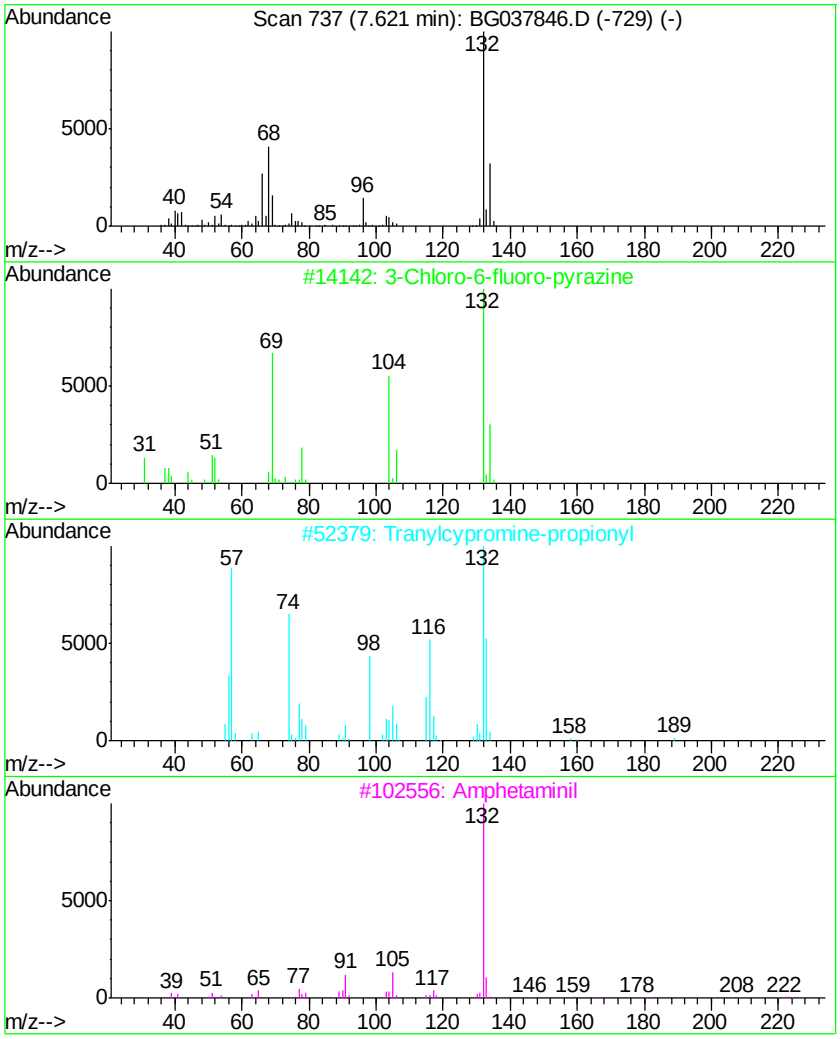
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

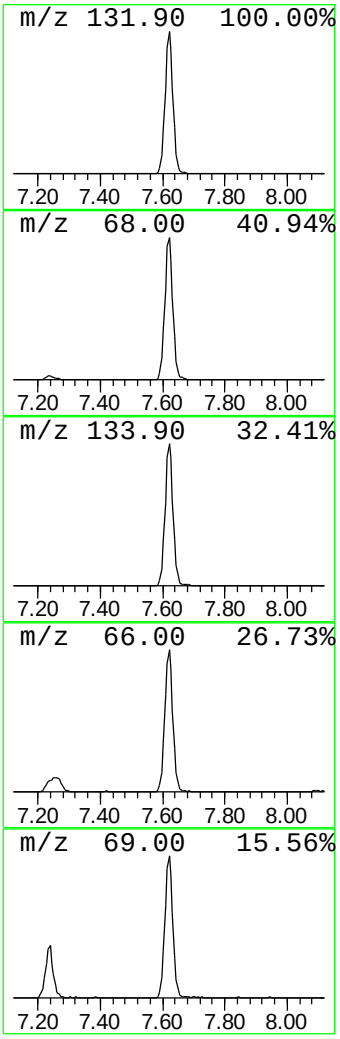
****

Peak Number 1 unknown7.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	73.17 ng	1189430	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110618\
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Operator : JU/SJ
Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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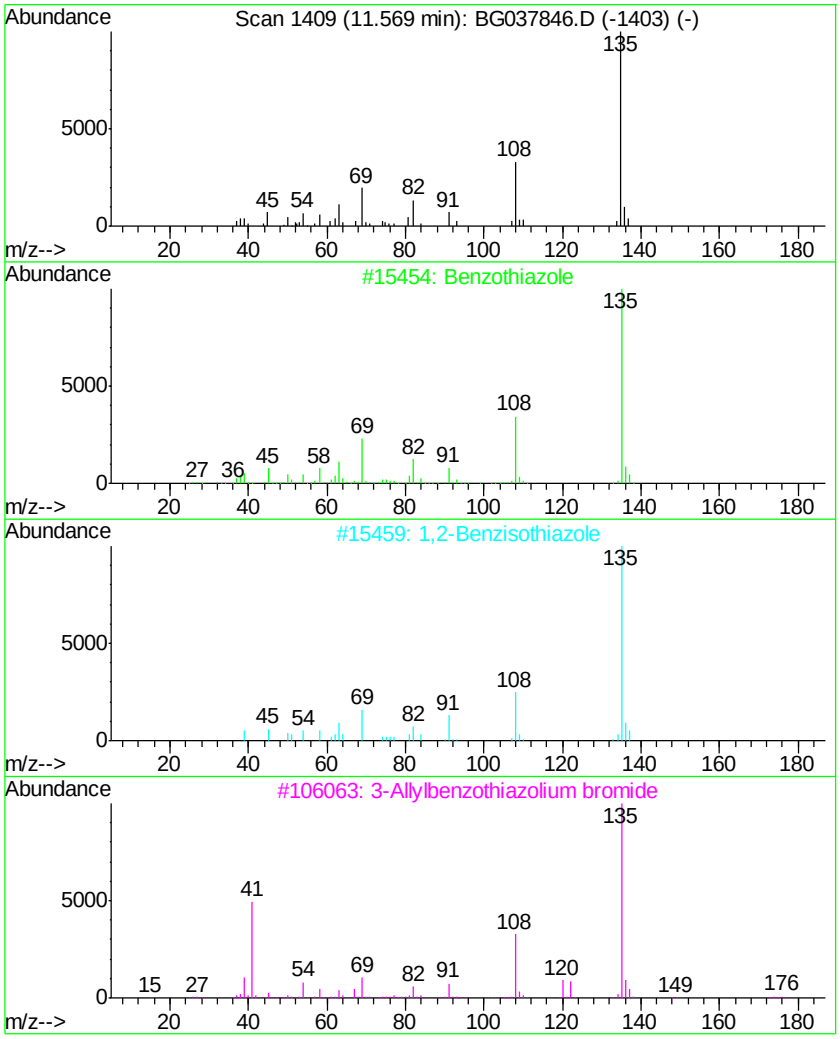
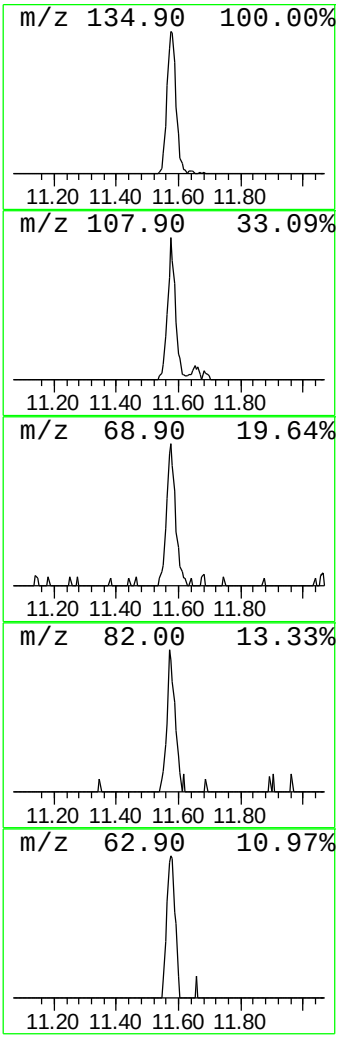
Peak Number 3 Benzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	3.36 ng	85977	Naphthalene-d8	10.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	94
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	80
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	74
4	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	59
5	Septacidin aminonucleoside	326	C12H18N6O5	003059-05-0	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110618\
Data File : BG037846.D
Acq On : 6 Nov 2018 20:02
Operator : JU/SJ
Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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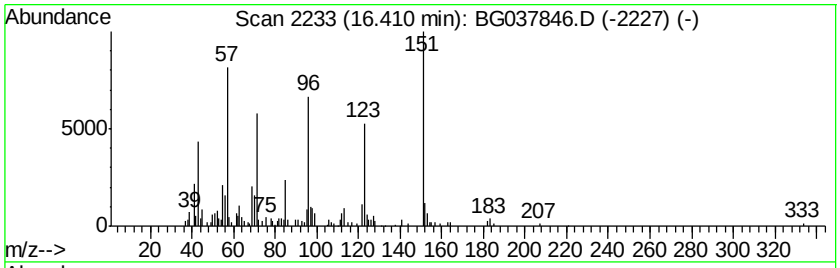
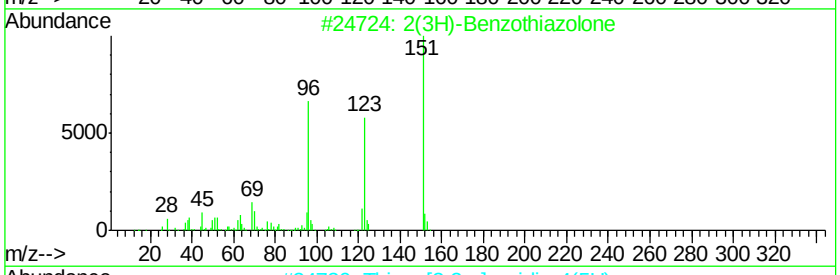
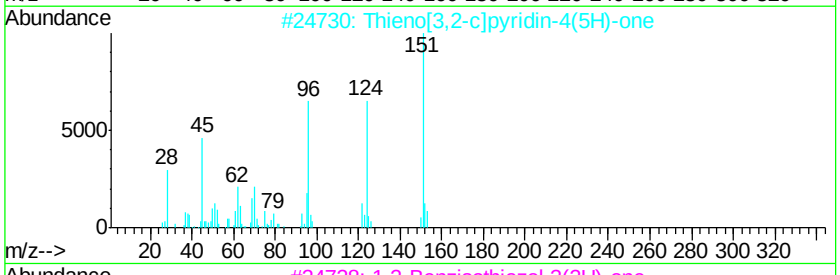
Peak Number 4 2(3H)-Benzothiazolone Concentration Rank 5

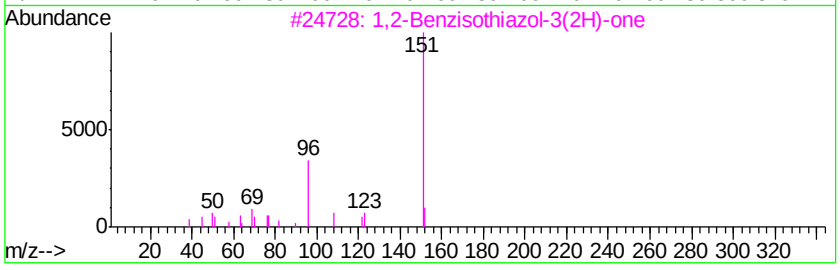
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	4.69 ng	191354	Phenanthrene-d10	17.47

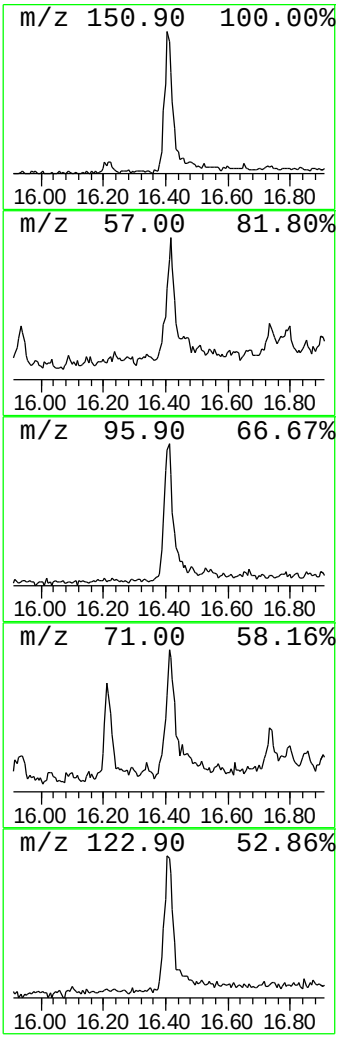
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	93
2	Thieno[3,2-c]pyridin-4(5H)-one	151	C7H5NOS	027685-92-3	46
3	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	43
4	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	38
5	Benzooxazole-2-thiol	151	C7H5NOS	1000318-31-6	22











Library Search Compound Report

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Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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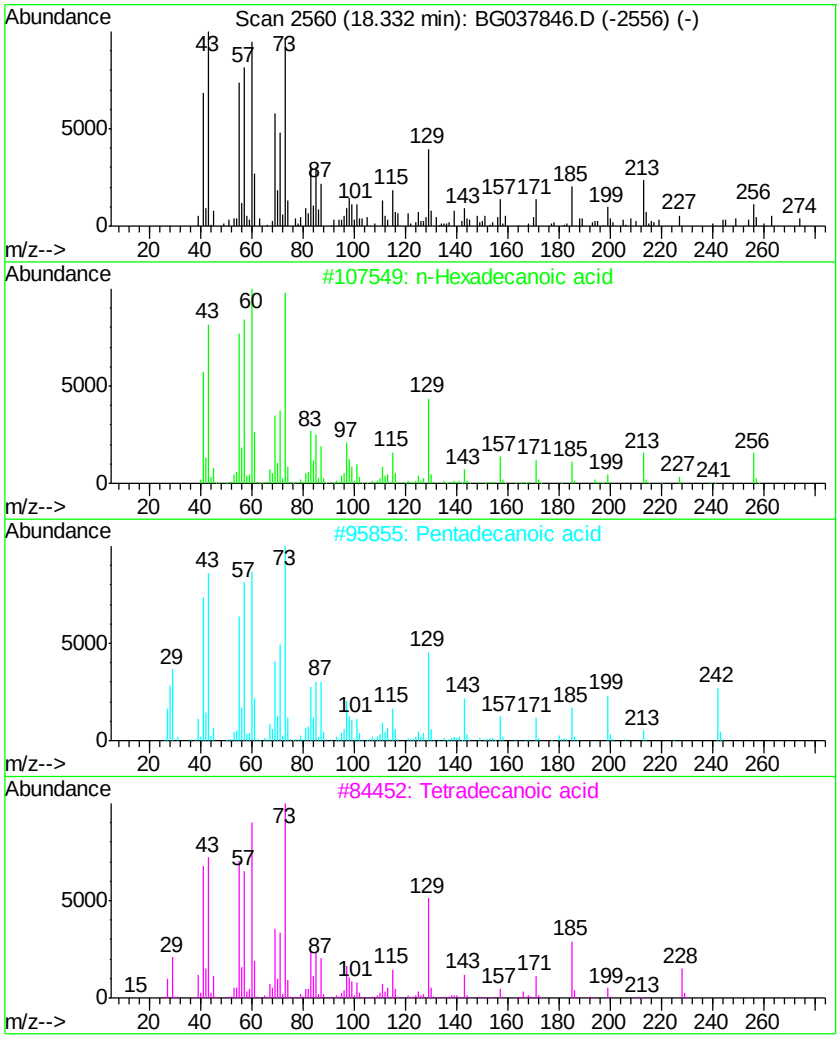
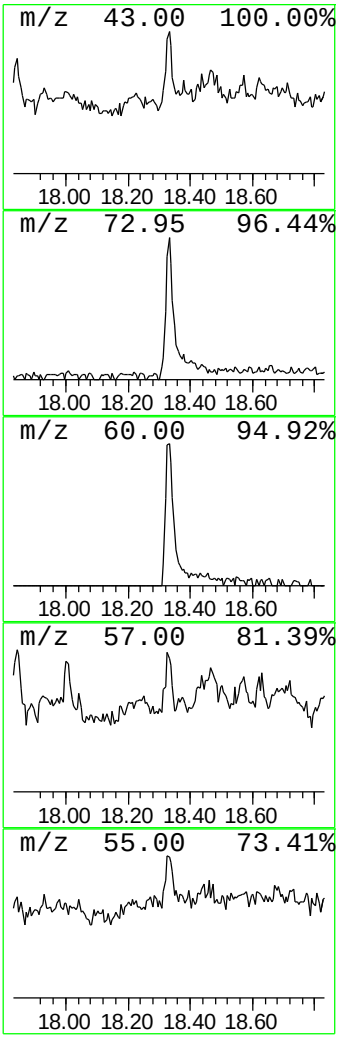
Peak Number 5 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	2.50 ng	101832	Phenanthrene-d10	17.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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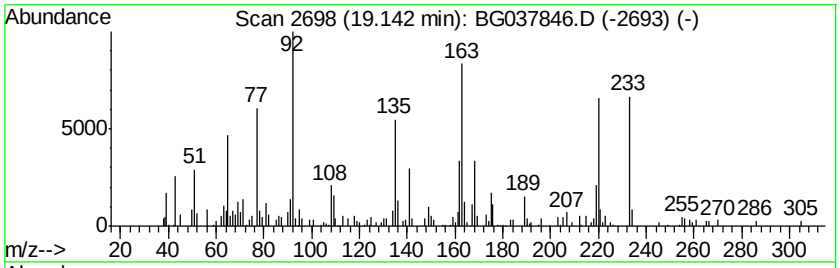
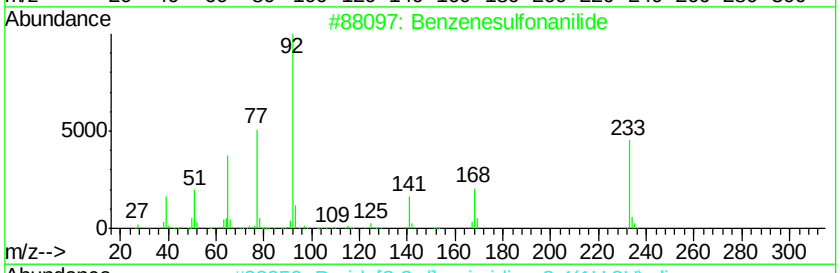
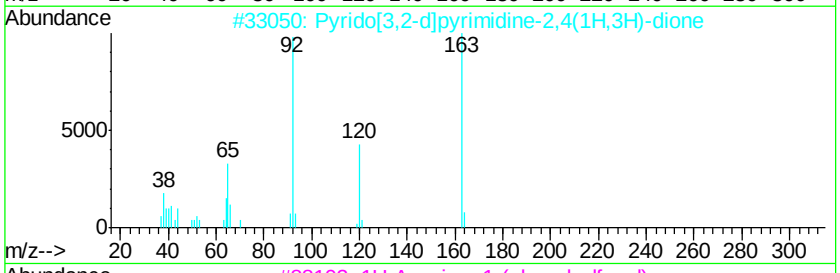
Peak Number 6 Benzenesulfonanilide Concentration Rank 7

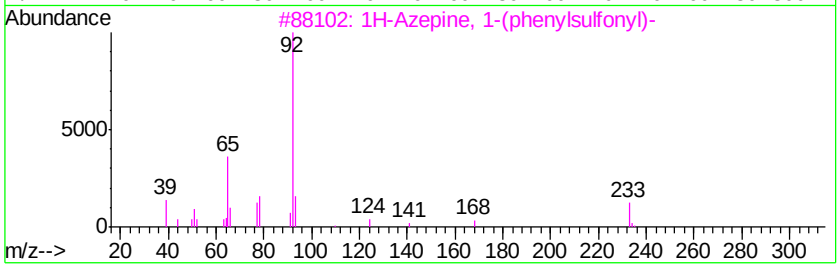
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.14	3.27 ng	133364	Phenanthrene-d10	17.47

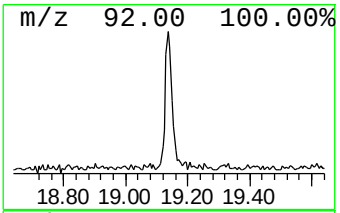
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonanilide	233	C12H11NO2S	001678-25-7	70
2	Pyrido[3,2-d]pyrimidine-2,4(1H,3...	163	C7H5N3O2	037538-68-4	53
3	1H-Azepine, 1-(phenylsulfonyl)-	233	C12H11NO2S	020646-54-2	43
4	Pyridine, 3-butyl-	135	C9H13N	000539-32-2	43
5	Pyrido[3,4-d]pyrimidine-2,4(1H,3...	163	C7H5N3O2	021038-67-5	35

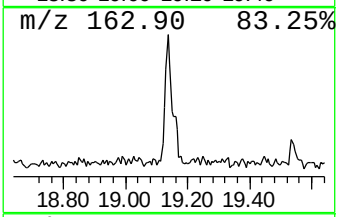


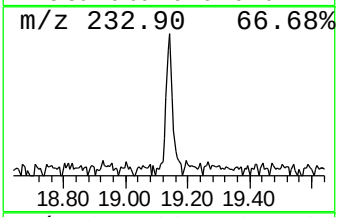


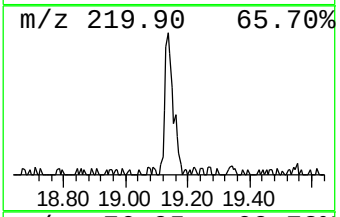


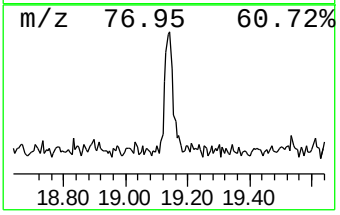












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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

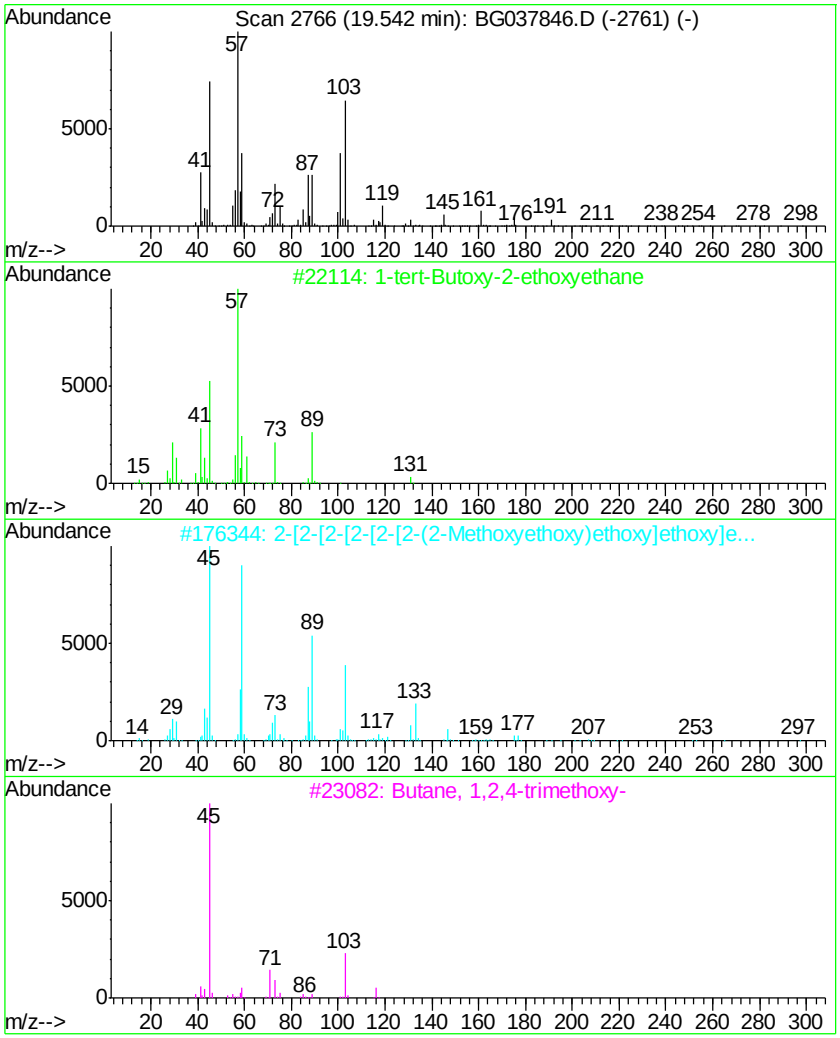
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

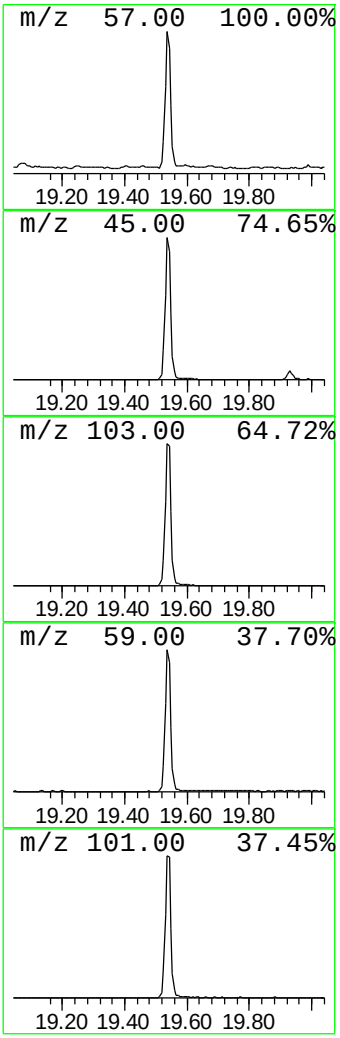
****

Peak Number 7 unknown19.54 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.54	29.33 ng	1196840	Phenanthrene-d10	17.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	43
2	2-[2-[2-[2-[2-[2-(2-Methoxyethox...	340	C15H32O8	1000352-04-1	38
3	Butane, 1,2,4-trimethoxy-	148	C7H16O3	020637-48-3	38
4	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	35
5	Butyl 2,5,8,11,14,17,20,23-octao...	454	C21H42O10	1000366-81-8	35





Library Search Compound Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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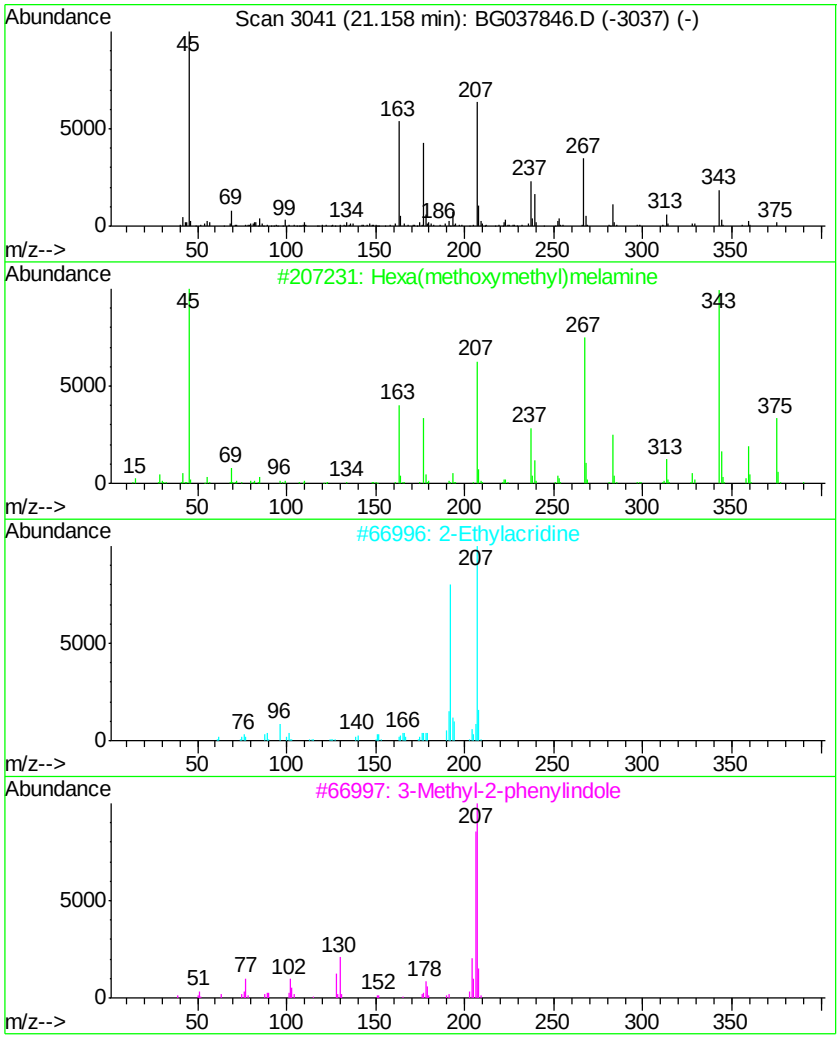
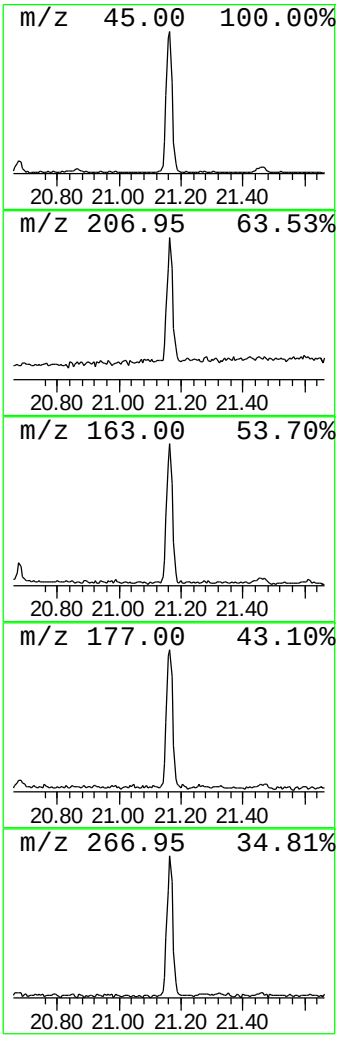
****

Peak Number 8 Hexa(methoxymethyl)melamine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.16	5.44 ng	220771	Chrysene-d12	21.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexa(methoxymethyl)melamine	390	C15H30N6O6	068002-20-0	56
2	2-Ethylacridine	207	C15H13N	055751-83-2	10
3	3-Methyl-2-phenylindole	207	C15H13N	010257-92-8	10
4	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	9
5	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110618\
Data File : BG037846.D
Acq On : 6 Nov 2018 20:02
Operator : JU/SJ
Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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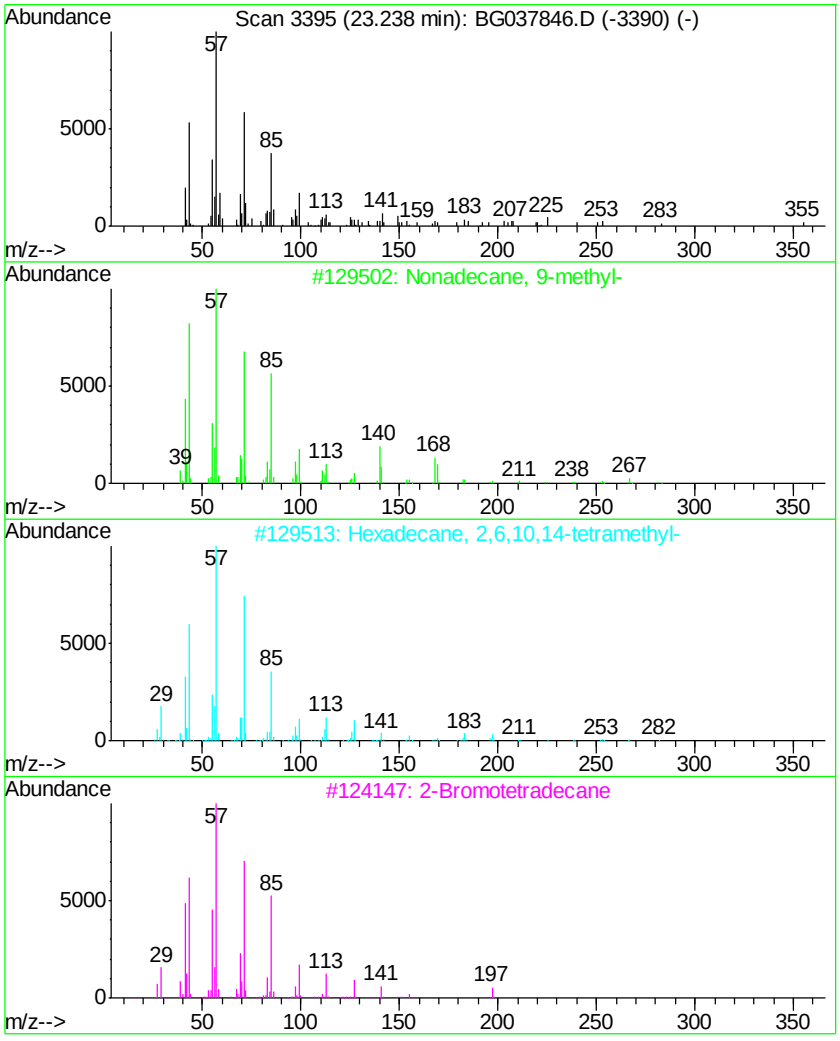
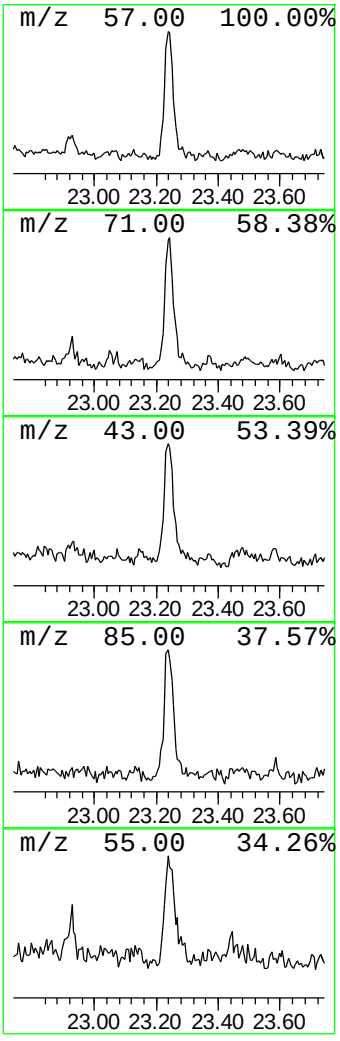
Peak Number 9 Nonadecane, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.24	3.15 ng	127750	Chrysene-d12	21.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	78
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	76
3	2-Bromotetradecane	276	C14H29Br	074036-95-6	64
4	Octadecane	254	C18H38	000593-45-3	64
5	Hexadecane	226	C16H34	000544-76-3	64





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Data File : BG037846.D
Acq On : 6 Nov 2018 20:02
Operator : JU/SJ
Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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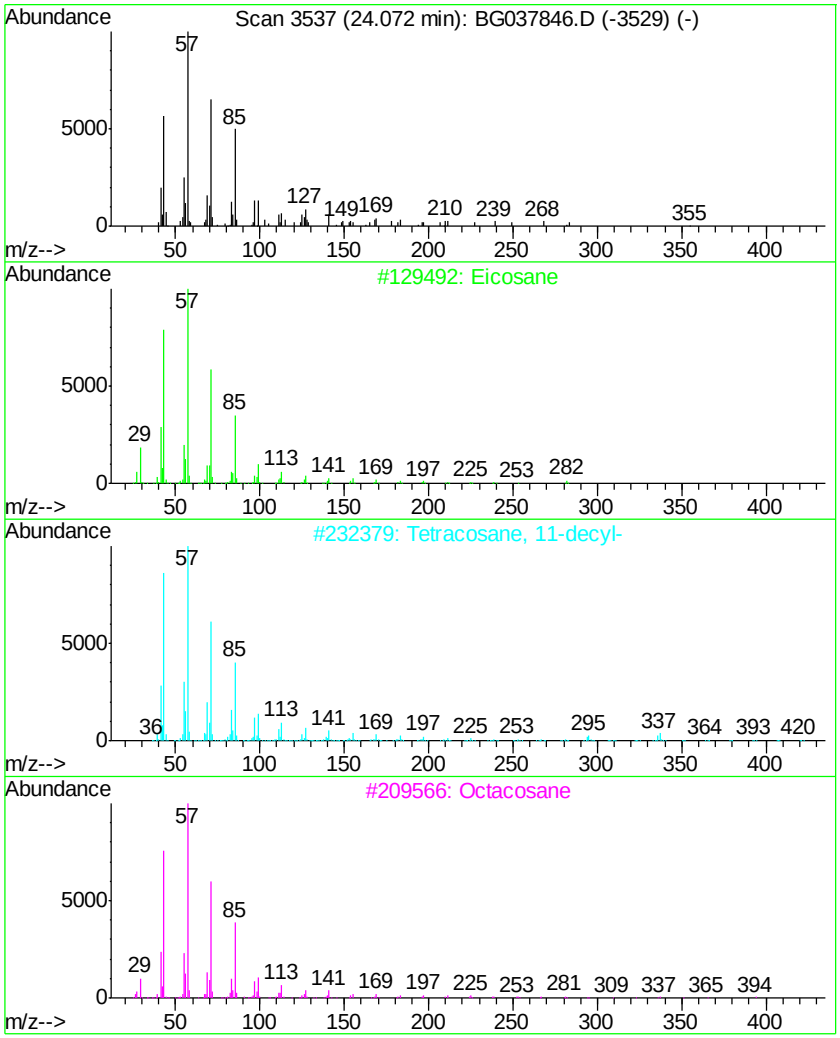
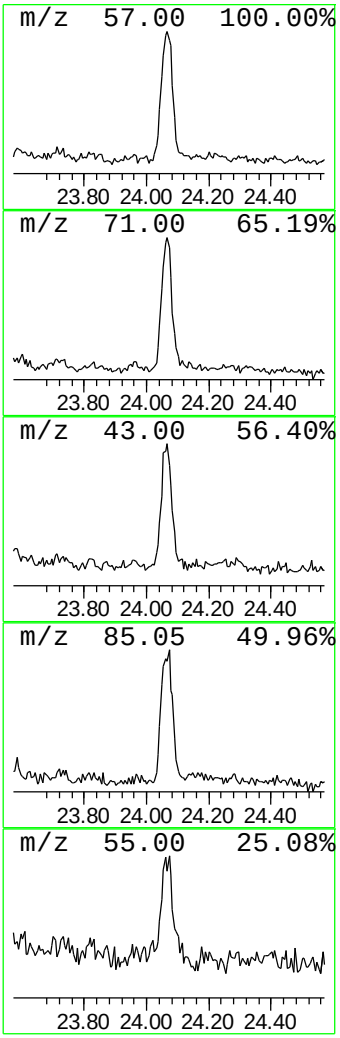
Peak Number 10 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.07	2.56 ng	106299	Perylene-d12	25.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
3	Octacosane	394	C28H58	000630-02-4	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110618\
Data File : BG037846.D
Acq On : 6 Nov 2018 20:02
Operator : JU/SJ
Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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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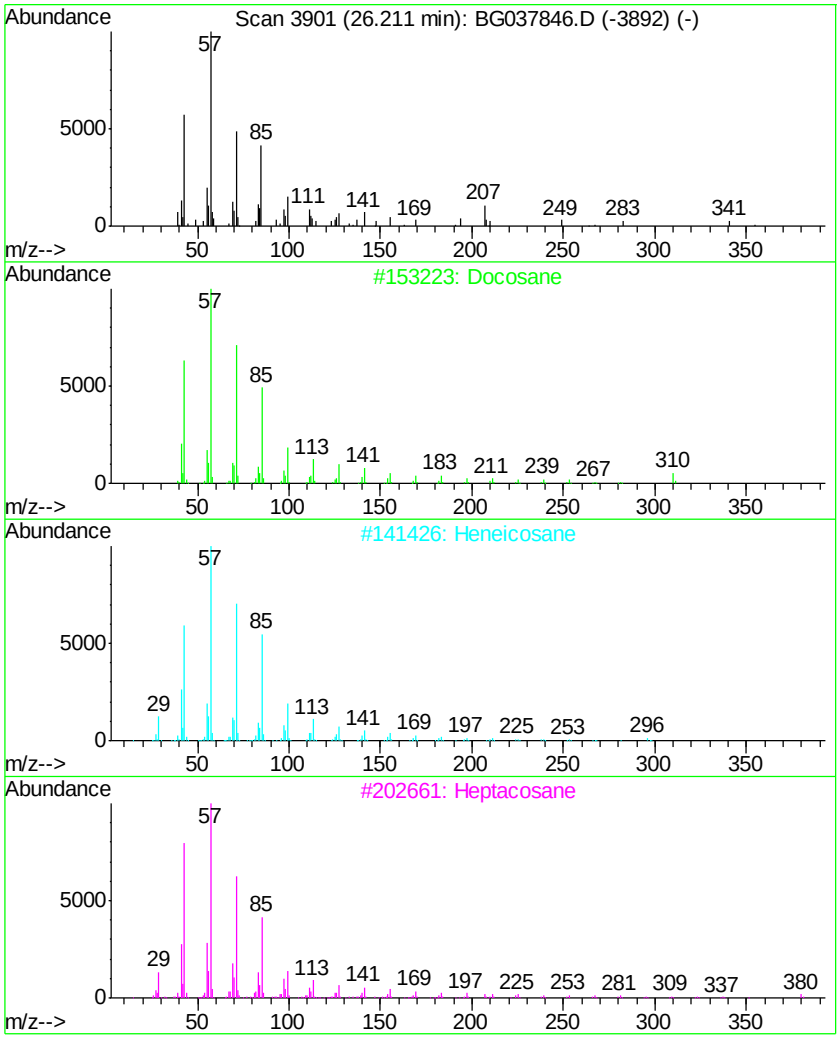
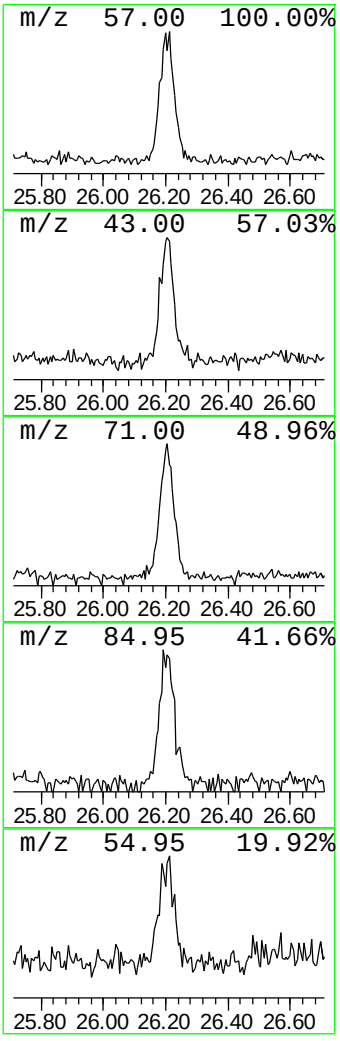
Peak Number 11 Docosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.21	2.15 ng	89221	Perylene-d12	25.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	74
2	Heneicosane	296	C21H44	000629-94-7	74
3	Heptacosane	380	C27H56	000593-49-7	74
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
5	Hentriacontane	437	C31H64	000630-04-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG110618\
Data File : BG037846.D
Acq On : 6 Nov 2018 20:02
Operator : JU/SJ
Sample : J5804-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BS-DRUM-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.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
unknown7.62	7.62	73.2	ng	1189430	1	8.10	325092	20.0
Benzothiazole	11.57	3.4	ng	85977	2	10.92	511343	20.0
2(3H)-Benzothiazo...	16.41	4.7	ng	191354	4	17.47	816049	20.0
n-Hexadecanoic acid	18.33	2.5	ng	101832	4	17.47	816049	20.0
Benzenesulfonanilide	19.14	3.3	ng	133364	4	17.47	816049	20.0
unknown19.54	19.54	29.3	ng	1196840	4	17.47	816049	20.0
Hexa(methoxymethy...	21.16	5.4	ng	220771	5	21.76	811774	20.0
Nonadecane, 9-met...	23.24	3.1	ng	127750	5	21.76	811774	20.0
Eicosane	24.07	2.6	ng	106299	6	25.09	831311	20.0
Docosane	26.21	2.1	ng	89221	6	25.09	831311	20.0