LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
Data File : BG028819.D
Acq On : 19 Sep 2017 7:01
Operator : SJ/JU
Sample : I5265-12
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-12D68

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-BG091217.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	5.389	300	306	312	rBV	67644	105557	3.53%	0.692%
2	5.859	378	386	396	rBV	642918	1088760	36.39%	7.141%
3	7.445	648	656	672	rBV	663352	1215168	40.62%	7.970%
4	7.821	712	720	730	rBV	636424	1119695	37.42%	7.344%
5	8.285	792	799	806	rBV	111408	196275	6.56%	1.287%
6	8.614	846	855	863	rBV2	361040	637666	21.31%	4.182%
7	9.460	991	999	1011	rBV	383923	695530	23.25%	4.562%
8	11.111	1271	1280	1292	rBV	155794	297069	9.93%	1.948%
9	13.526	1683	1691	1703	rBV	925598	1465356	48.98%	9.611%
10	14.343	1823	1830	1839	rBV	122271	187464	6.27%	1.230%
11	14.907	1919	1926	1936	rBV2	286823	477835	15.97%	3.134%
12	16.399	2173	2180	2190	rBV	1119111	1773017	59.26%	11.629%
13	17.657	2387	2394	2401	rBV2	421041	673646	22.52%	4.418%
14	18.509	2535	2539	2549	rBV4	51195	92888	3.10%	0.609%
15	18.990	2615	2621	2626	rBV2	58183	80544	2.69%	0.528%
16	19.413	2688	2693	2697	rVV	79318	95486	3.19%	0.626%
17	19.484	2700	2705	2710	rVB4	26892	36202	1.21%	0.237%
18	19.772	2750	2754	2759	rBV4	24824	40937	1.37%	0.269%
19	20.248	2828	2835	2842	rBV	2253400	2991905	100.00%	19.624%
20	20.518	2876	2881	2885	rBV	73228	87371	2.92%	0.573%
21	20.882	2936	2943	2948	rBV8	23557	43679	1.46%	0.286%
22	21.558	3052	3058	3069	rBV3	77438	189910	6.35%	1.246%
23	21.981	3123	3130	3141	rBV	424530	798130	26.68%	5.235%
24	22.569	3224	3230	3237	rBV3	18981	37922	1.27%	0.249%
25	23.503	3384	3389	3399	rVB4	26334	61777	2.06%	0.405%
26	25.447	3708	3720	3737	rBV2	234099	756700	25.29%	4.963%

Sum of corrected areas: 15246489

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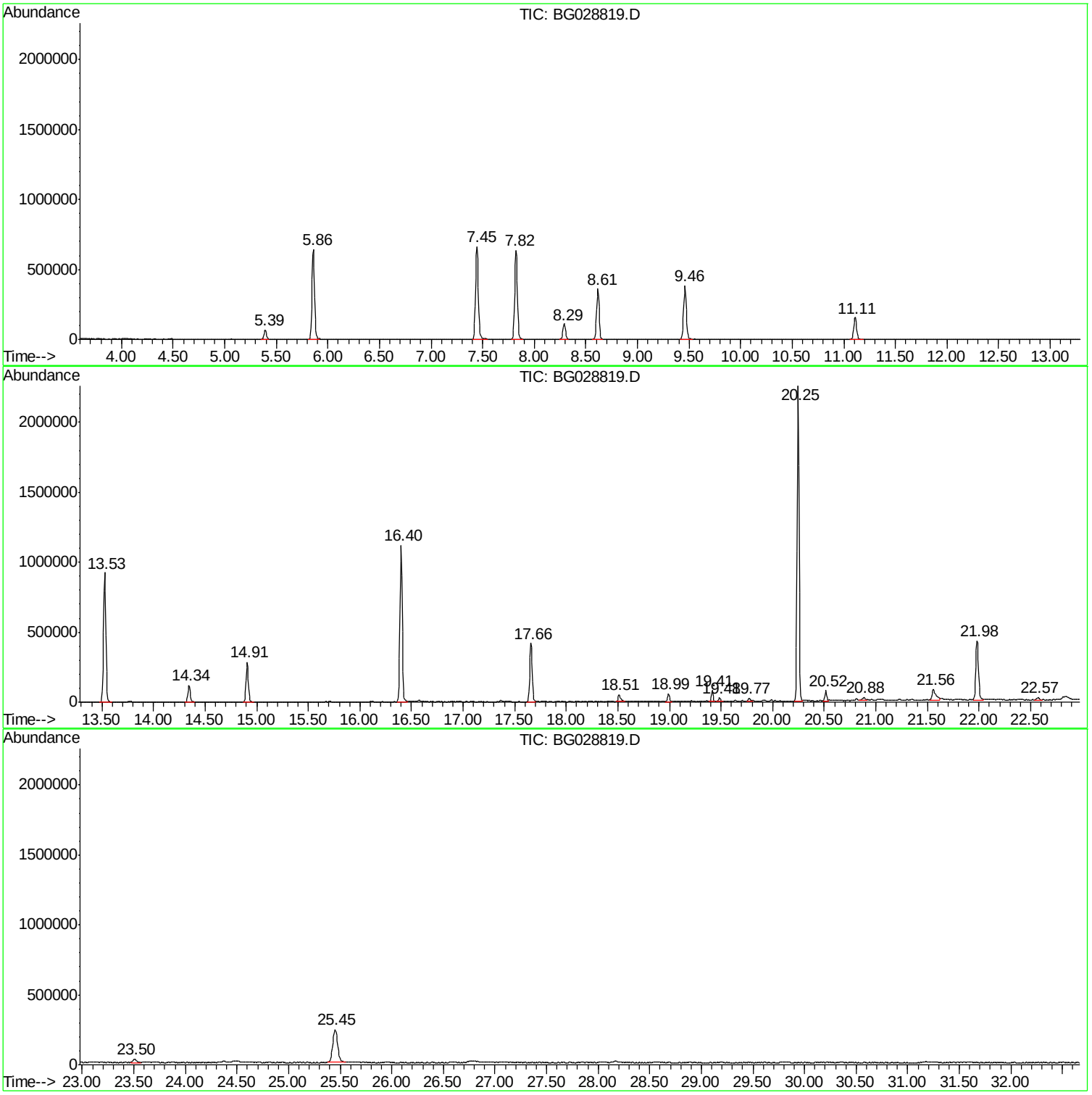
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 27 Sample Multiplier: 1

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TIC Library : C:\Database\NIST11.L
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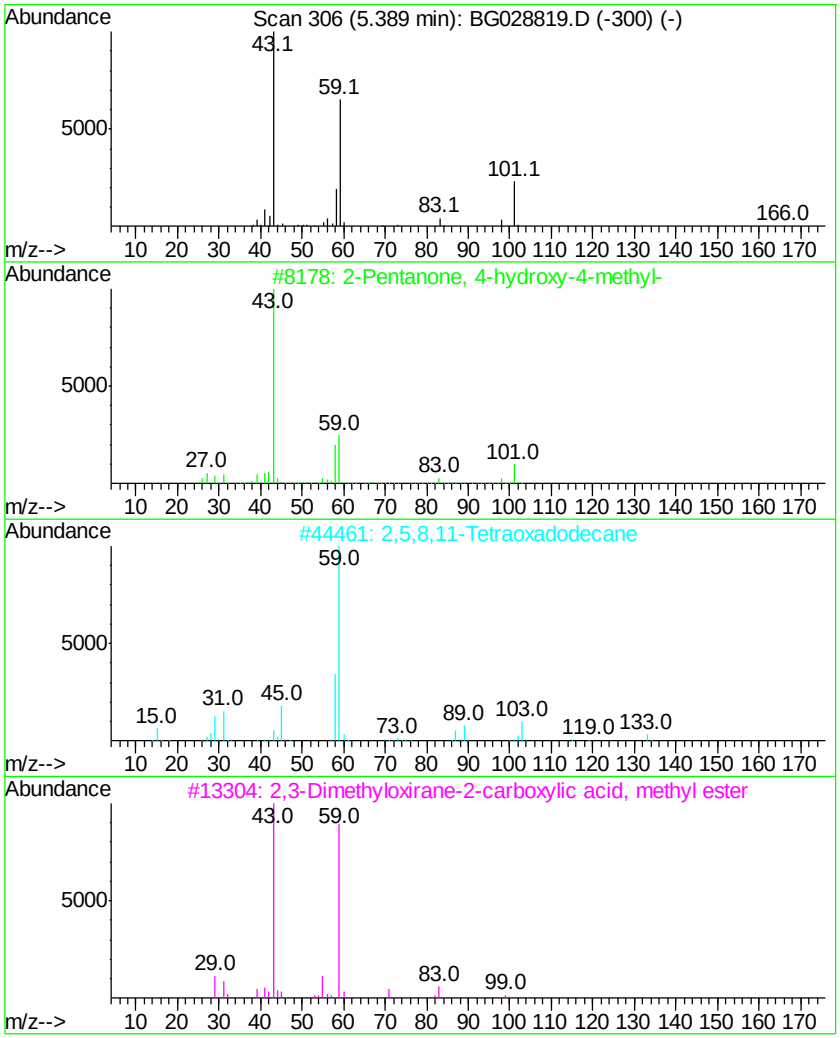
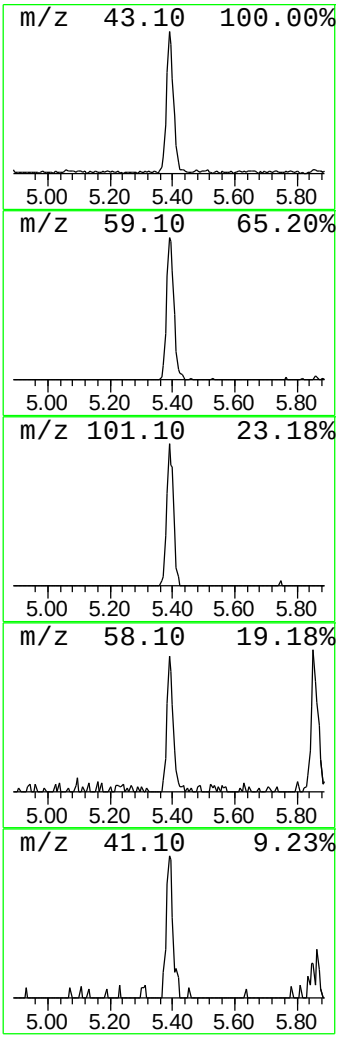
Peak Number 1 unknown5.39 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.39	10.76 ng	105557	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	25
3	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	25
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG091817\
Data File : BG028819.D
Acq On : 19 Sep 2017 7:01
Operator : SJ/JU
Sample : I5265-12
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-12D68

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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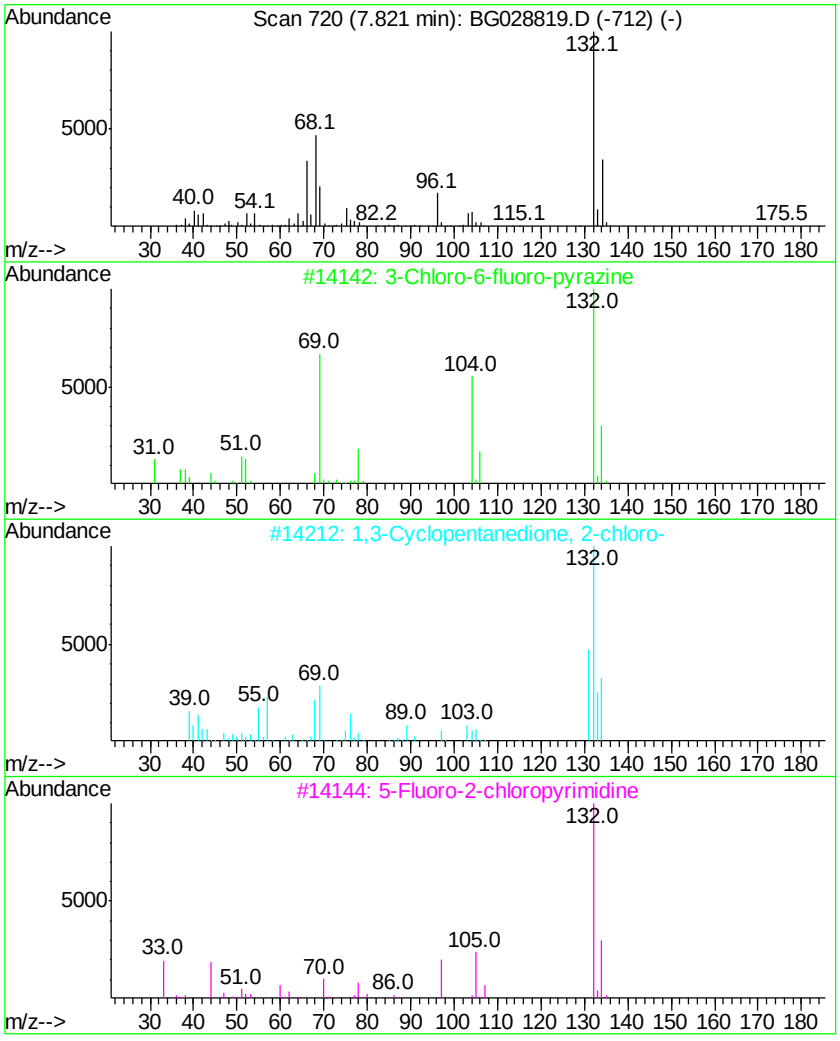
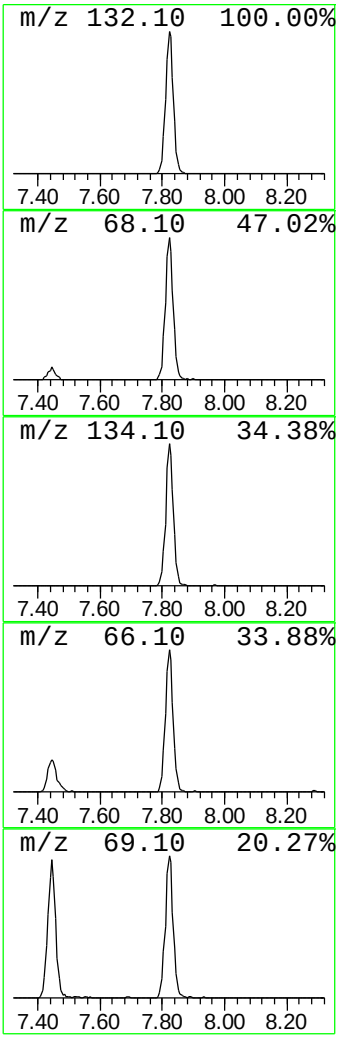
Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	114.10 ng	1119700	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Operator : SJ/JU
Sample : I5265-12
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-12D68

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
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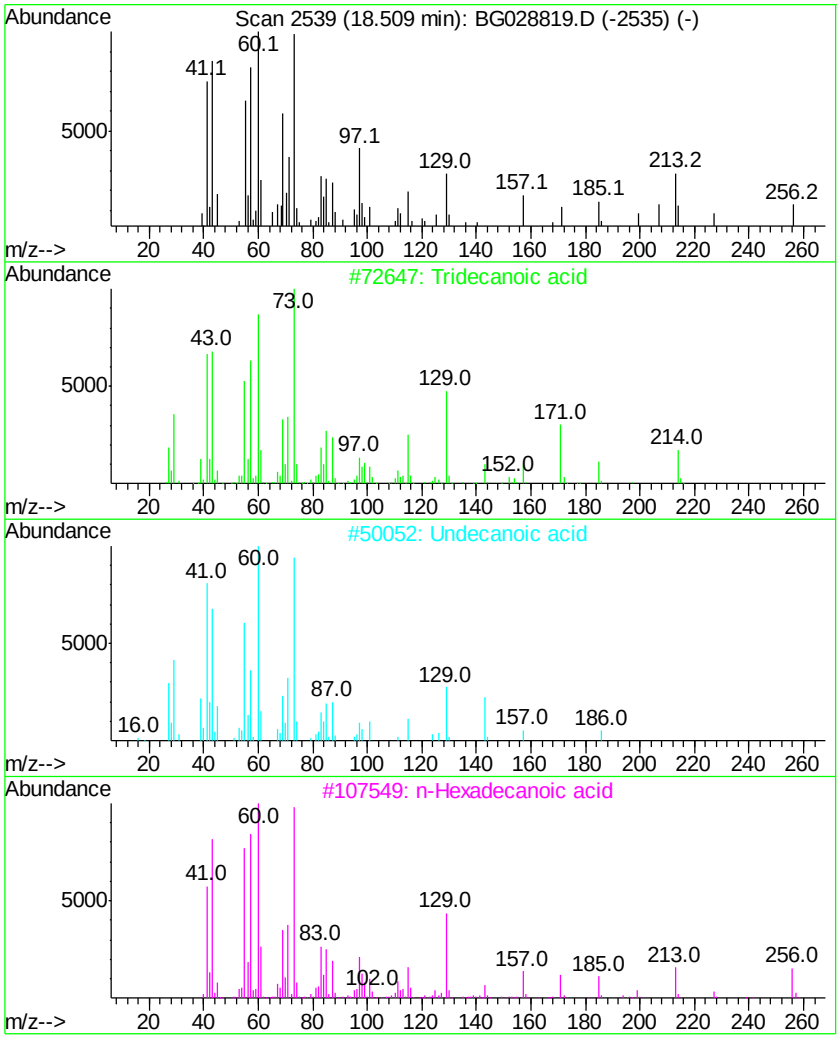
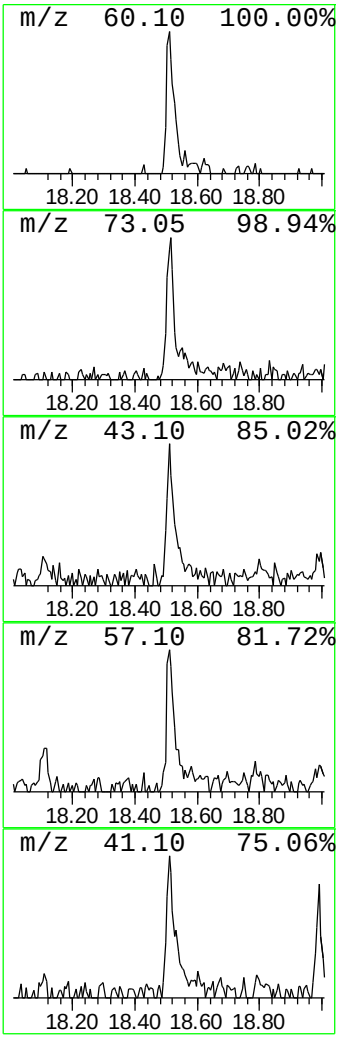
Peak Number 4 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.51	2.76 ng	92888	Phenanthrene-d10	17.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	76
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	50





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Sample : I5265-12
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-12D68

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
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TIC Library : C:\Database\NIST11.L
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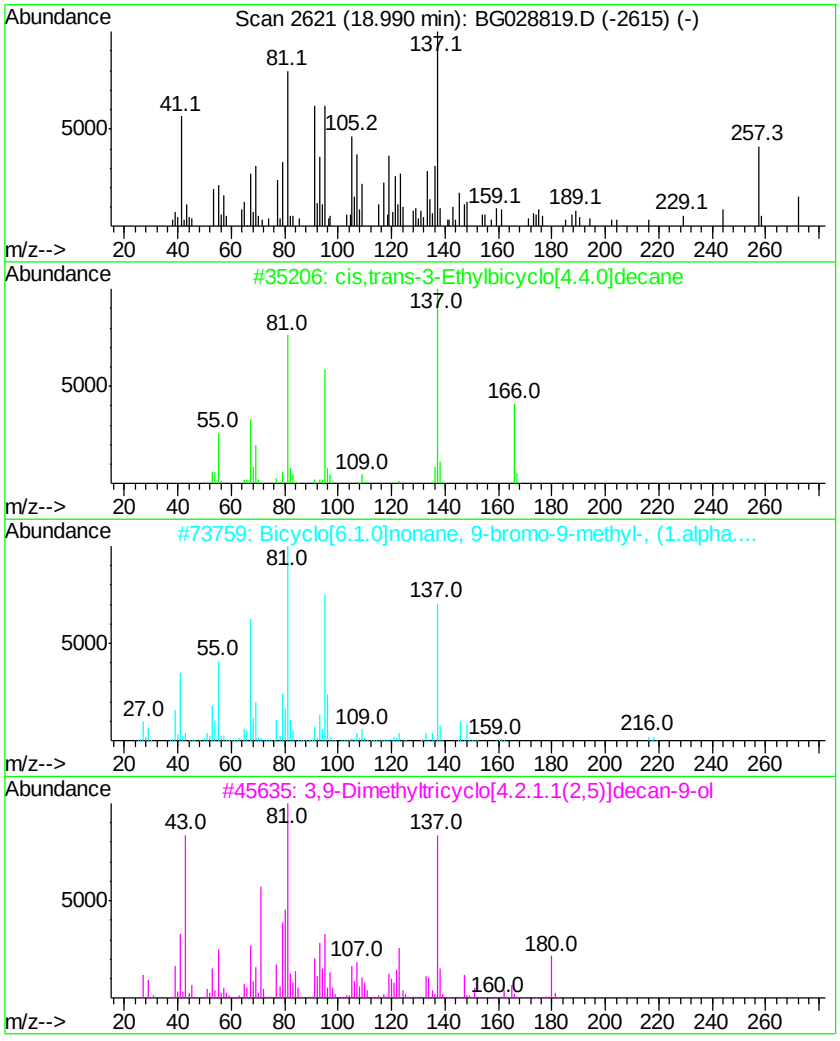
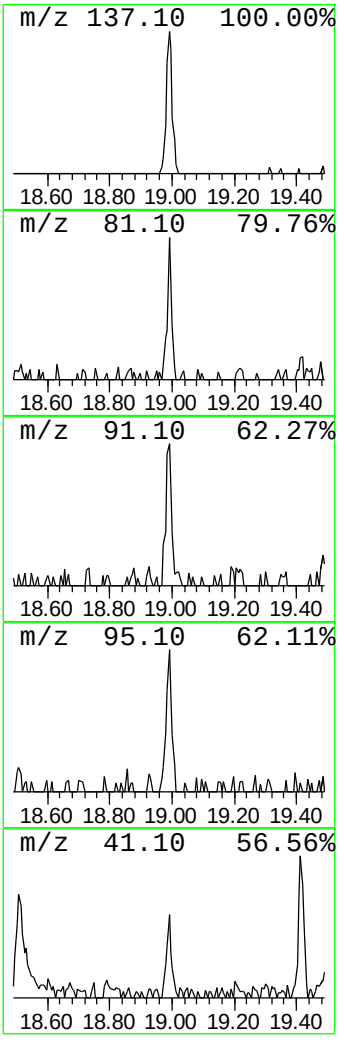
Peak Number 5 unknown18.99 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.99	2.39 ng	80544	Phenanthrene-d10	17.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,trans-3-Ethylbicyclo[4.4.0]d...	166	C12H22	066660-41-1	47
2	Bicyclo[6.1.0]nonane, 9-bromo-9-...	216	C10H17Br	059474-03-2	47
3	3,9-Dimethyltricyclo[4.2.1.1(2,5...	180	C12H20O	1000185-61-6	35
4	4-Dimethylaminopyridin-2-amine	137	C7H11N3	050426-31-8	14
5	2,6-Pyridinedicarboxylic acid, d...	195	C9H9NO4	005453-67-8	14





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Instrument : BNA_G
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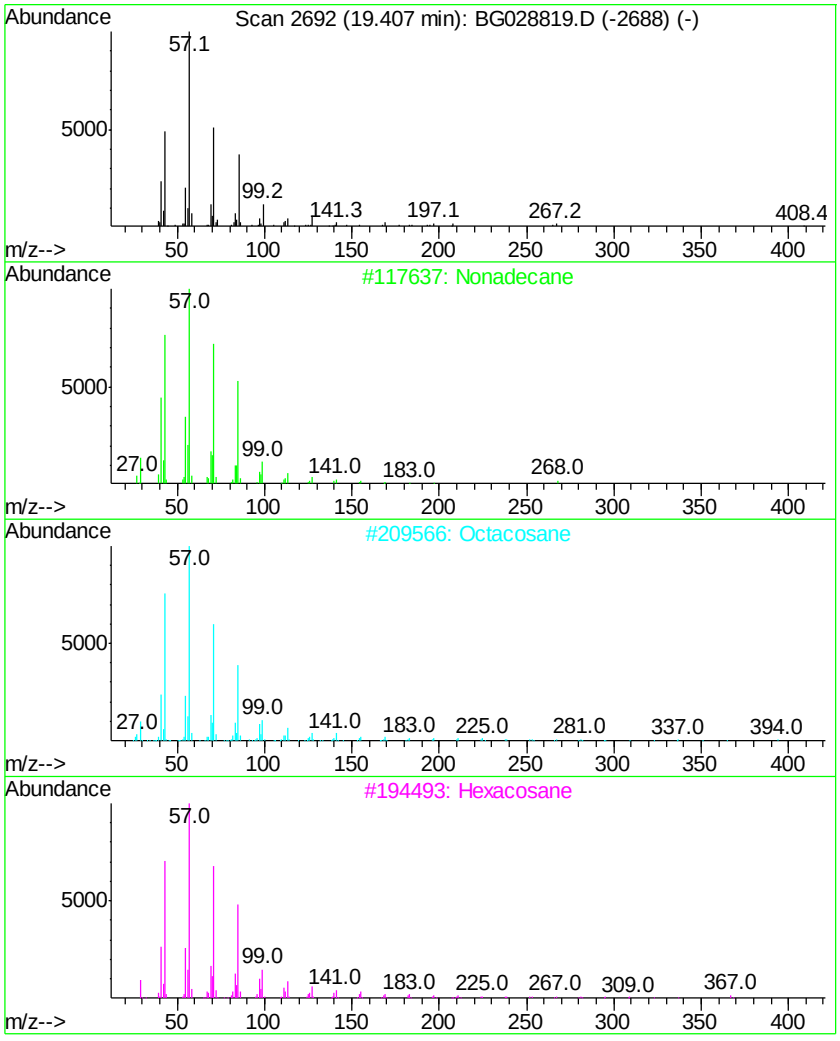
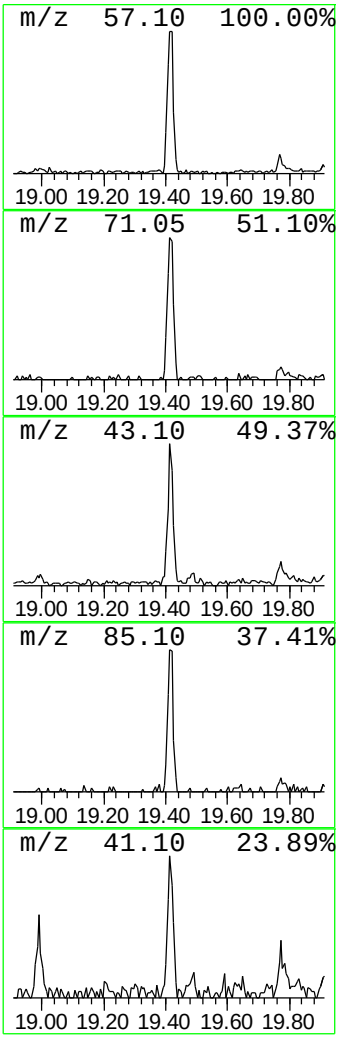
Peak Number 6 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.41	2.83 ng	95486	Phenanthrene-d10	17.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Hexacosane	366	C26H54	000630-01-3	86
4	Tetracosane	338	C24H50	000646-31-1	86
5	Heneicosane	296	C21H44	000629-94-7	83





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Instrument : BNA_G
ClientSampleId : TP-12D68

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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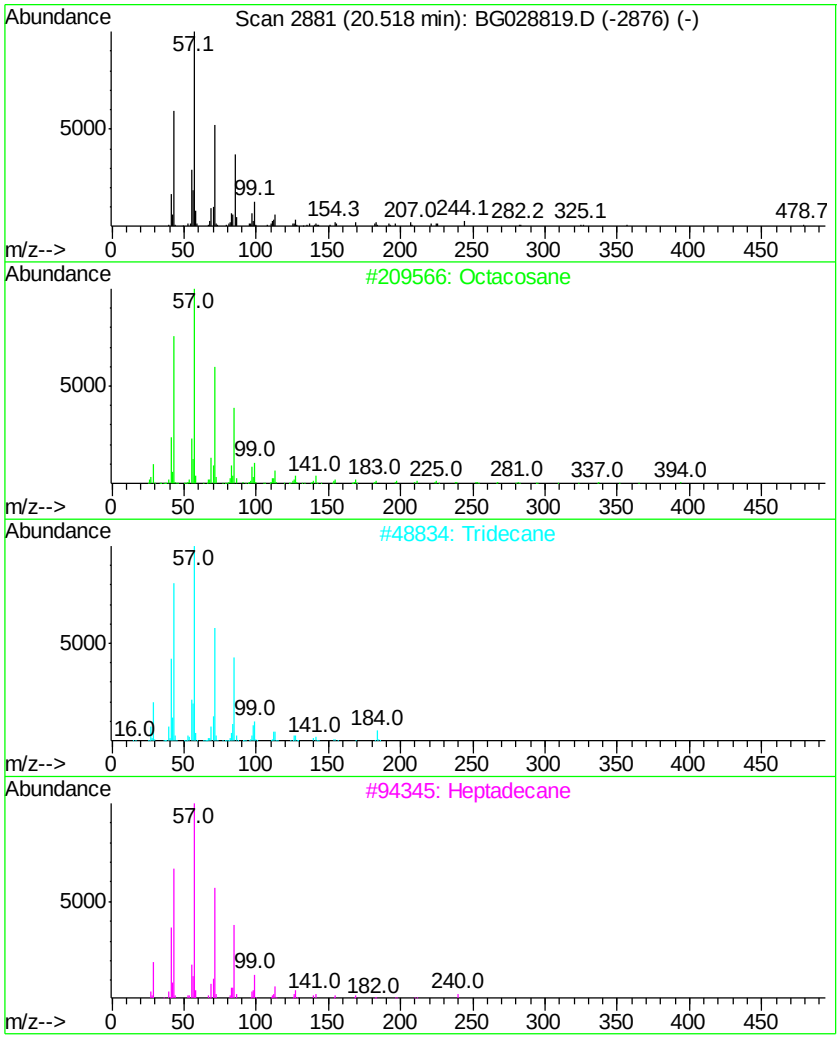
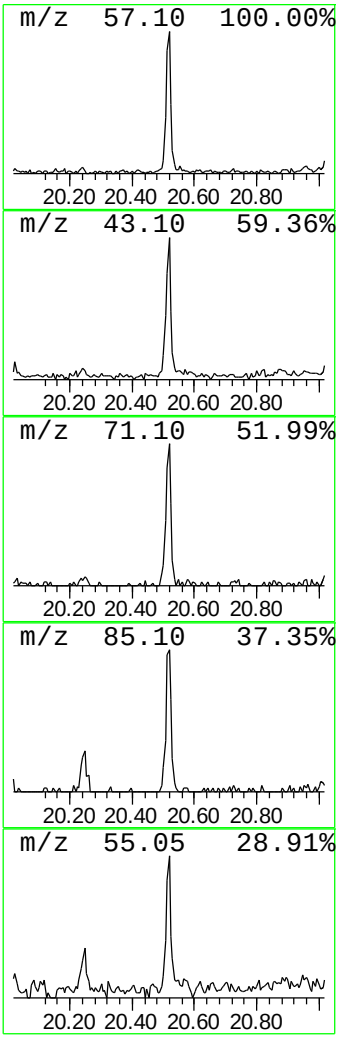
Peak Number 7 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.52	2.19 ng	87371	Chrysene-d12	21.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	83
2	Tridecane	184	C13H28	000629-50-5	80
3	Heptadecane	240	C17H36	000629-78-7	80
4	Eicosane	282	C20H42	000112-95-8	76
5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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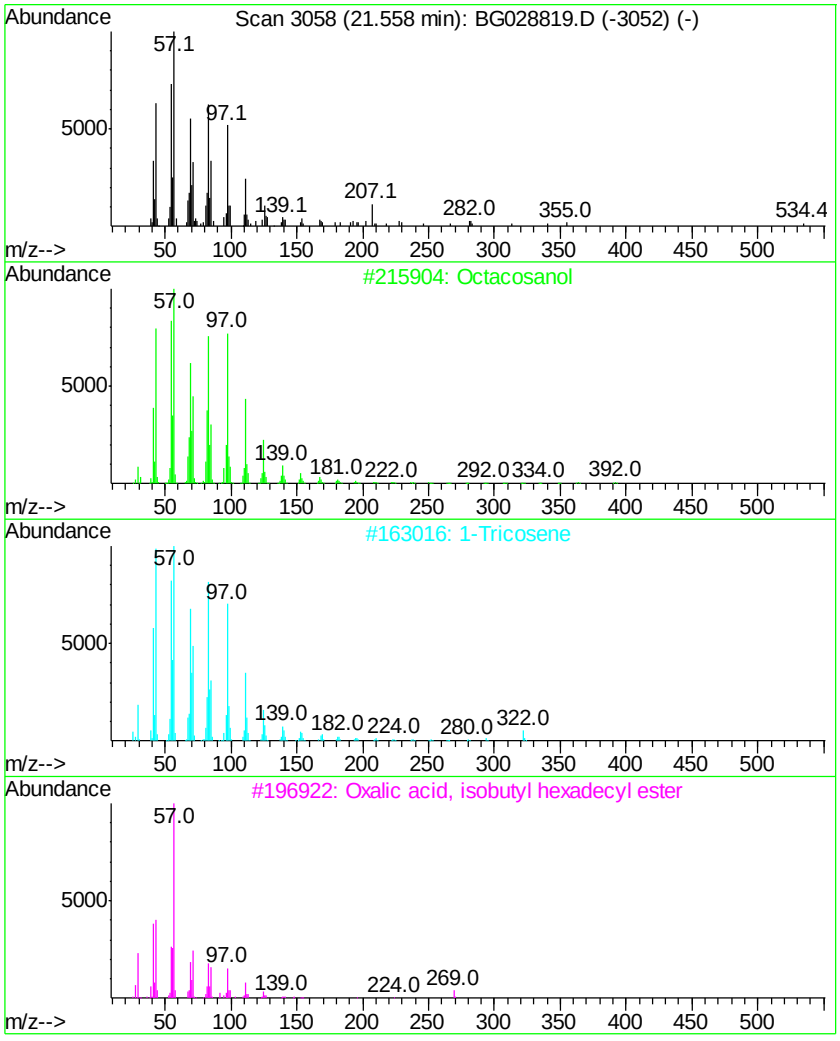
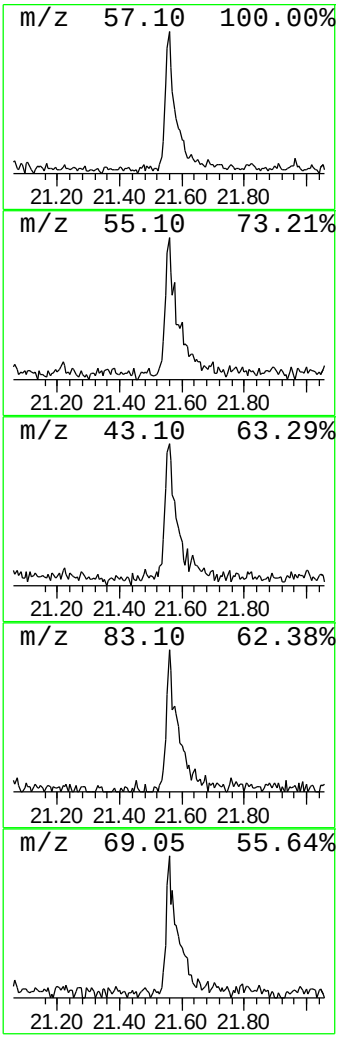
Peak Number 8 Octacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.56	4.76 ng	189910	Chrysene-d12	21.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	81
2	1-Tricosene	322	C23H46	018835-32-0	74
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	72
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	70
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	70





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.39	5.39	10.8	ng	105557	1	8.29	196275	20.0
unknown7.82	7.82	114.1	ng	1119700	1	8.29	196275	20.0
Tridecanoic acid	18.51	2.8	ng	92888	4	17.66	673646	20.0
unknown18.99	18.99	2.4	ng	80544	4	17.66	673646	20.0
Nonadecane	19.41	2.8	ng	95486	4	17.66	673646	20.0
Octacosane	20.52	2.2	ng	87371	5	21.98	798130	20.0
Octacosanol	21.56	4.8	ng	189910	5	21.98	798130	20.0