LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023422.D
Acq On : 3 Aug 2016 12:19
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9524

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-BG080116.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	2.994	21	26	39	rVB	3393545	4927917	19.43%	1.683%
2	5.185	394	399	406	rBV	170191	258720	1.02%	0.088%
3	5.667	474	481	492	rVB	771619	1282481	5.06%	0.438%
4	7.282	746	756	757	rBV	992611	1507973	5.95%	0.515%
5	7.306	757	760	770	rVB	1298870	2134504	8.42%	0.729%
6	7.535	793	799	805	rVB	388144	608636	2.40%	0.208%
7	7.652	812	819	835	rVB2	867363	2011377	7.93%	0.687%
8	8.010	872	880	887	rBV2	330876	564915	2.23%	0.193%
9	8.122	892	899	910	rVV2	388302	662319	2.61%	0.226%
10	8.451	948	955	962	rBV	660699	1140184	4.50%	0.389%
11	8.574	968	976	986	rBV	1144275	1998300	7.88%	0.683%
12	8.898	1024	1031	1034	rBV	1343877	2378065	9.38%	0.812%
13	8.933	1034	1037	1044	rVB	1862236	2926973	11.54%	1.000%
14	9.297	1091	1099	1107	rBV	576487	1054326	4.16%	0.360%
15	9.867	1186	1196	1204	rBV	2259072	3918652	15.45%	1.339%
16	10.061	1221	1229	1237	rBV	999407	1784509	7.04%	0.610%
17	10.601	1314	1321	1334	rBV	2054445	3766614	14.85%	1.287%
18	10.818	1350	1358	1367	rBV	2355943	4194056	16.53%	1.433%
19	10.959	1370	1382	1385	rBV	565820	1052492	4.15%	0.360%
20	11.006	1385	1390	1400	rVB	1310402	2405150	9.48%	0.822%
21	11.283	1429	1437	1445	rBV	1596593	2729256	10.76%	0.932%
22	12.234	1591	1599	1614	rBV	898536	1599124	6.30%	0.546%
23	12.610	1655	1663	1673	rBV	2146146	3511066	13.84%	1.199%
24	13.292	1772	1779	1790	rBV	2593074	4357799	17.18%	1.489%
25	13.403	1790	1798	1807	rVB	2197742	3492299	13.77%	1.193%
26	13.662	1831	1842	1847	rBV	1021379	1653293	6.52%	0.565%
27	14.231	1932	1939	1945	rVB	392374	629624	2.48%	0.215%
28	14.361	1954	1961	1969	rBV	3120727	4839075	19.08%	1.653%
29	14.508	1979	1986	1999	rVB	1606189	2641519	10.41%	0.902%
30	14.784	2026	2033	2040	rBV2	1050210	1719433	6.78%	0.587%
31	15.013	2065	2072	2084	rBV	1208155	2303974	9.08%	0.787%
32	15.148	2090	2095	2097	rBV	1265445	1813016	7.15%	0.619%
33	15.189	2097	2102	2111	rVB	7330079	12703117	50.08%	4.339%
34	15.600	2162	2172	2180	rBV	7836622	11954937	47.13%	4.084%

LSC Area Percent Report

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Data File : BG023422.D
Acq On : 3 Aug 2016 12:19
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9524

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-BG080116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.829	2202	2211	2224	rVB3	12081381	22645019	89.28%	7.736%
36	16.282	2282	2288	2299	rBV	2783903	4287861	16.90%	1.465%
37	16.722	2357	2363	2371	rBV	2559358	3705241	14.61%	1.266%
38	16.857	2376	2386	2392	rBV	9795412	15899838	62.68%	5.431%
39	17.198	2436	2444	2451	rBV	1105767	1742945	6.87%	0.595%
40	17.545	2495	2503	2509	rBV2	1430300	2330987	9.19%	0.796%
41	17.680	2518	2526	2534	rBV	3300192	5279329	20.81%	1.803%
42	18.420	2646	2652	2659	rBV	485035	746055	2.94%	0.255%
43	18.496	2659	2665	2670	rVB	4103038	5718603	22.55%	1.954%
44	19.601	2840	2853	2863	rBV	4060537	6139965	24.21%	2.097%
45	19.683	2863	2867	2874	rBV2	223462	297902	1.17%	0.102%
46	19.971	2907	2916	2922	rBV	9076711	15019880	59.22%	5.131%
47	20.153	2941	2947	2953	rBV	5713702	7647153	30.15%	2.612%
48	21.469	3166	3171	3179	rBV3	189009	435530	1.72%	0.149%
49	21.851	3227	3236	3242	rBV2	8356422	18333037	72.28%	6.263%
50	21.915	3242	3247	3256	rVB	5150073	9056241	35.70%	3.094%
51	23.589	3526	3532	3542	rVB	230685	491554	1.94%	0.168%
52	24.177	3620	3632	3638	rBV	4817158	14474372	57.06%	4.945%
53	24.253	3638	3645	3655	rVB2	5226751	13807927	54.44%	4.717%
54	25.087	3776	3787	3800	rVB	2405289	6716957	26.48%	2.295%
55	25.240	3803	3813	3824	rVB2	832573	2486236	9.80%	0.849%
56	26.421	4007	4014	4026	rVB3	156344	482590	1.90%	0.165%
57	29.229	4455	4492	4507	rBV	4214955	25364839	100.00%	8.665%
58	30.374	4663	4687	4704	rVB3	2317071	13098496	51.64%	4.475%

Sum of corrected areas: 292734252

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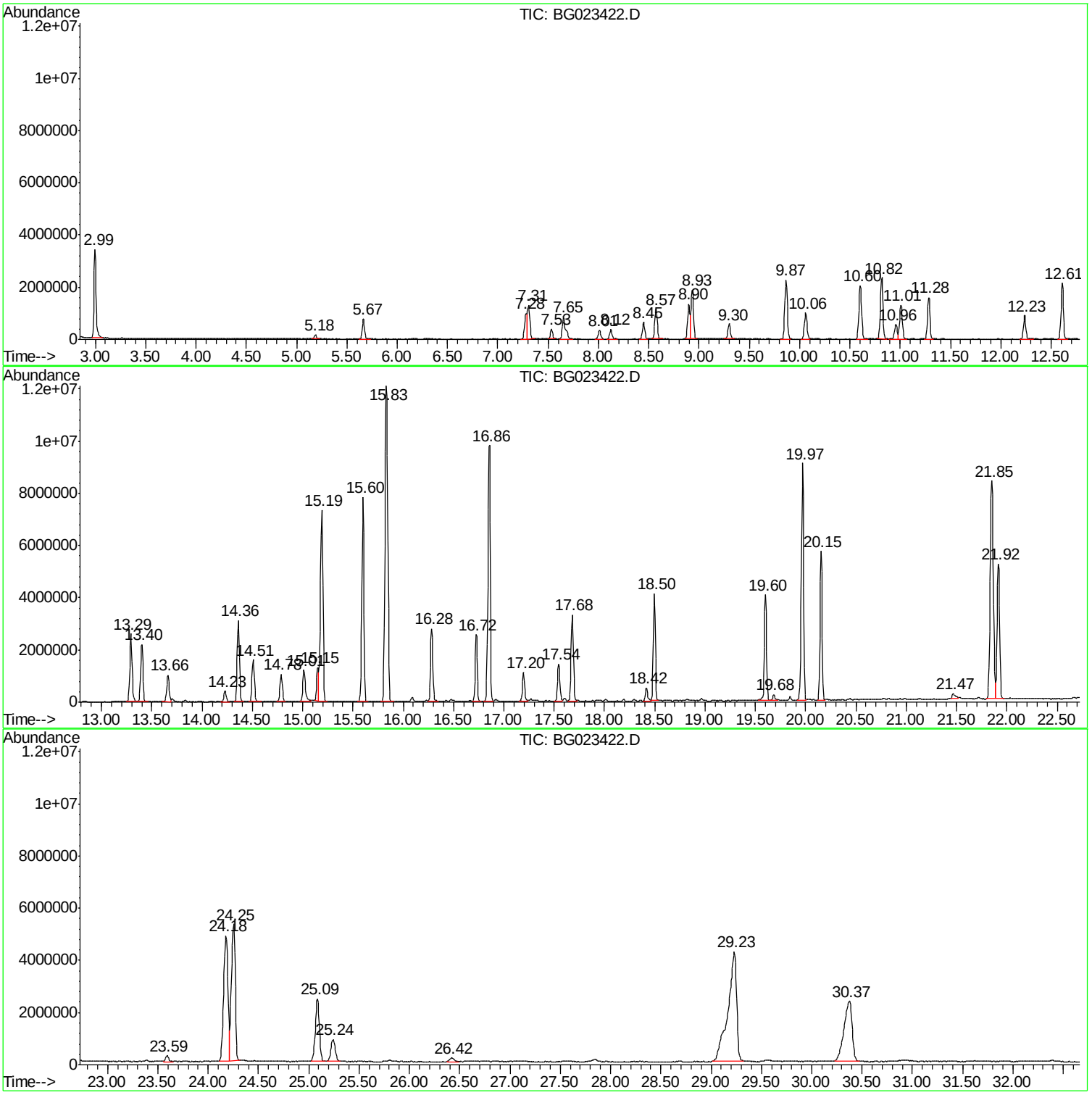
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
9524

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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\BG080316\
Data File : BG023422.D
Acq On : 3 Aug 2016 12:19
Operator : UM/SJ
Sample : H4145-18
Misc :
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Instrument : BNA_G
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

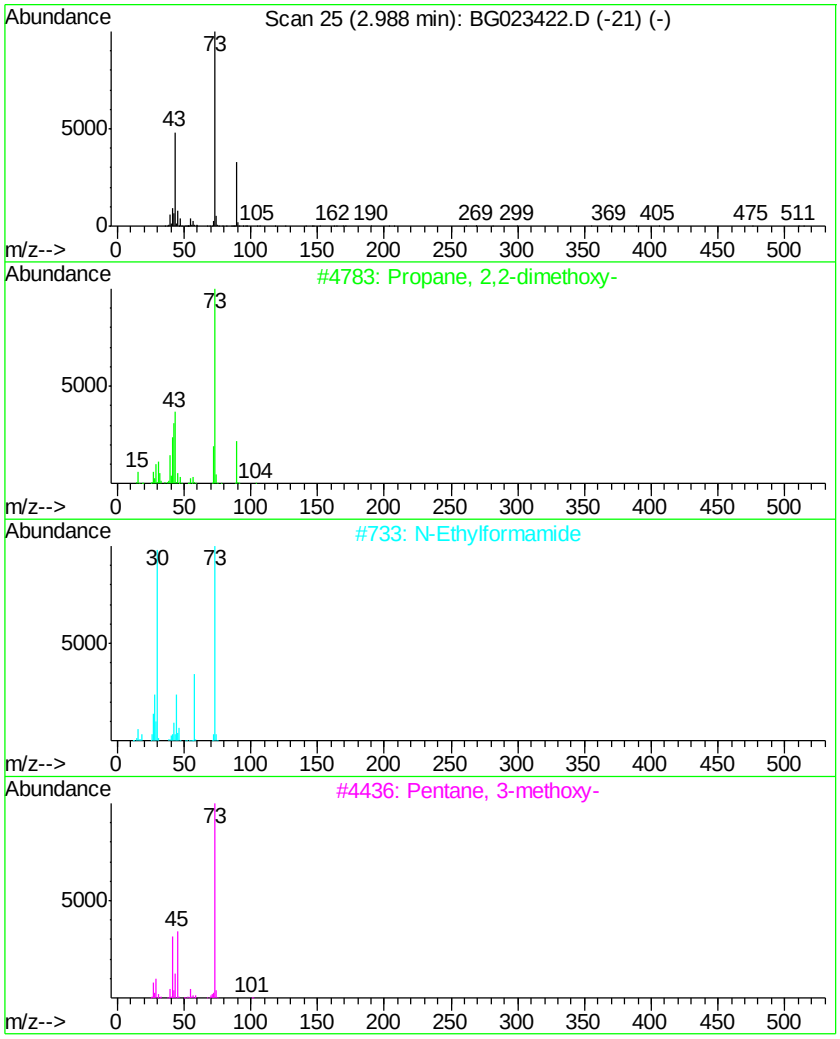
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

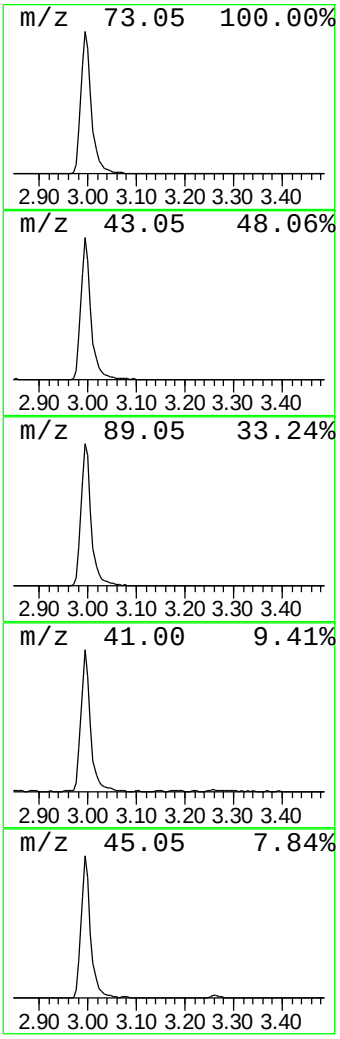
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	148.81 ng	4927920	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023422.D
Acq On : 3 Aug 2016 12:19
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

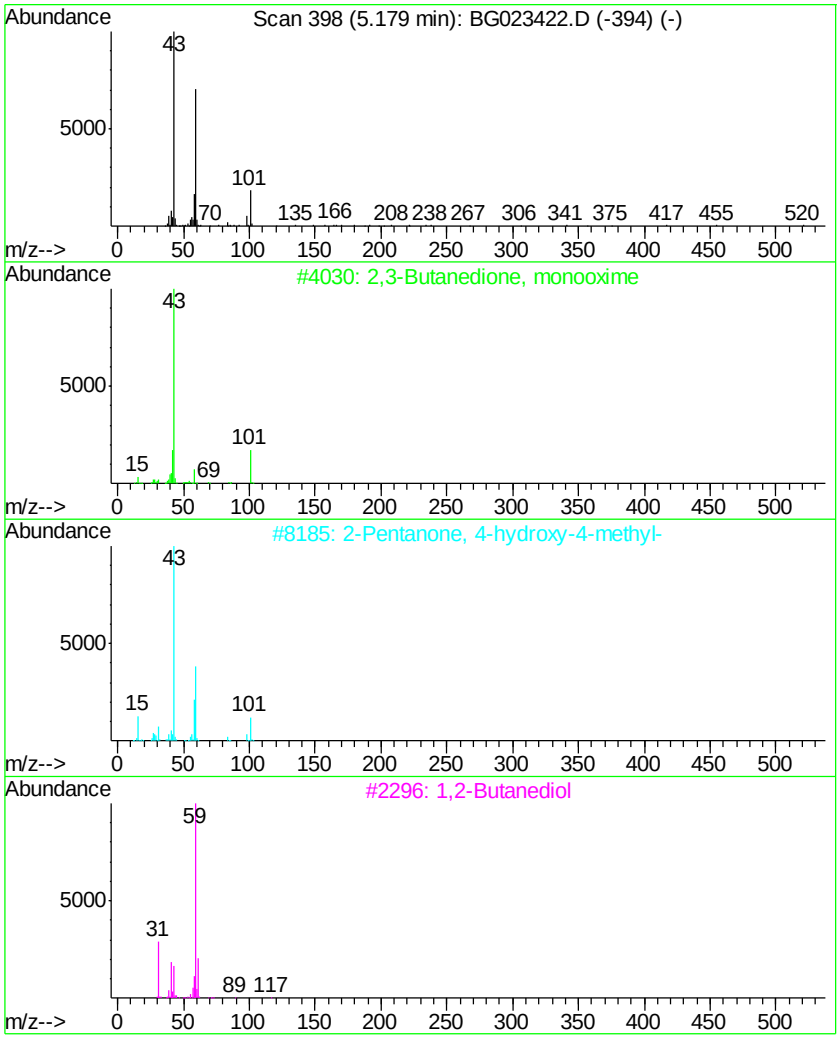
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

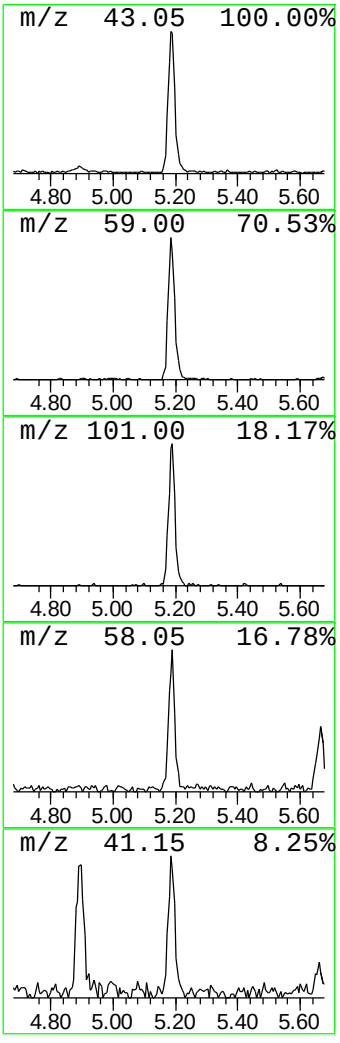
****

Peak Number 2 unknown5.18 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	7.81 ng	258720	1,4-Dichlorobenzene-d4	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32
3	1,2-Butanediol	90	C4H10O2	000584-03-2	23
4	1,1-Dimethyl-2-[2-(methoxycarbon...	160	C7H16N2O2	097812-30-1	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023422.D
Acq On : 3 Aug 2016 12:19
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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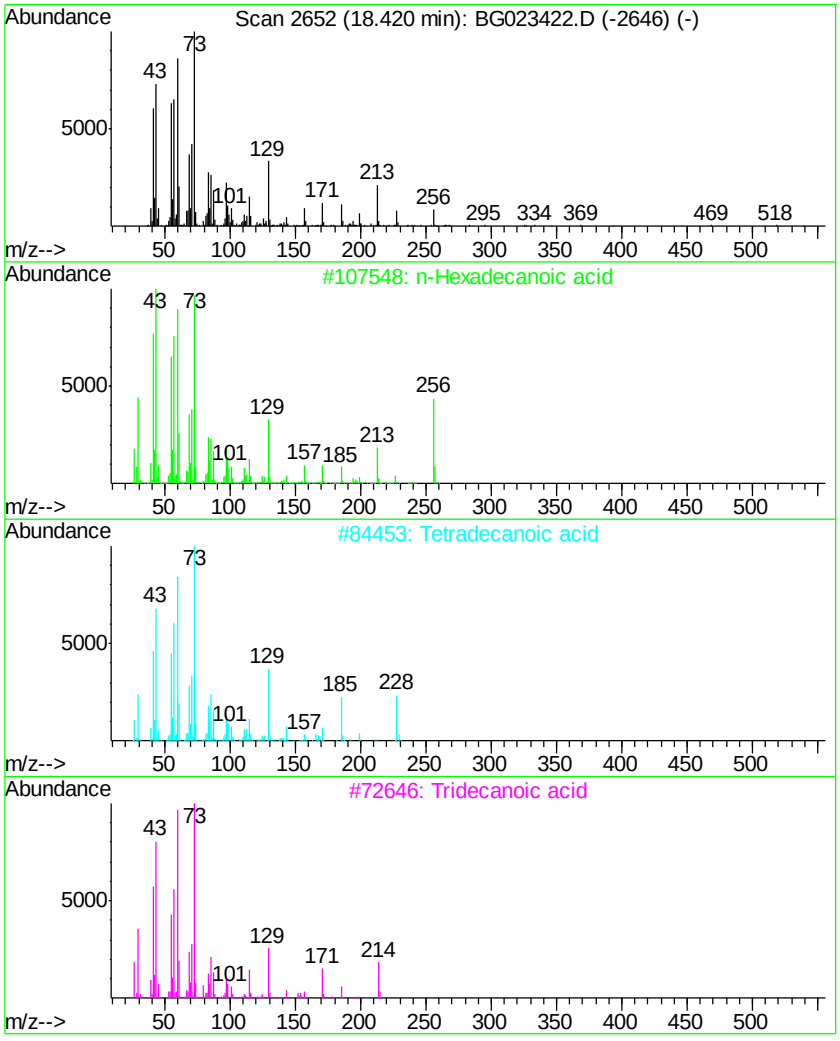
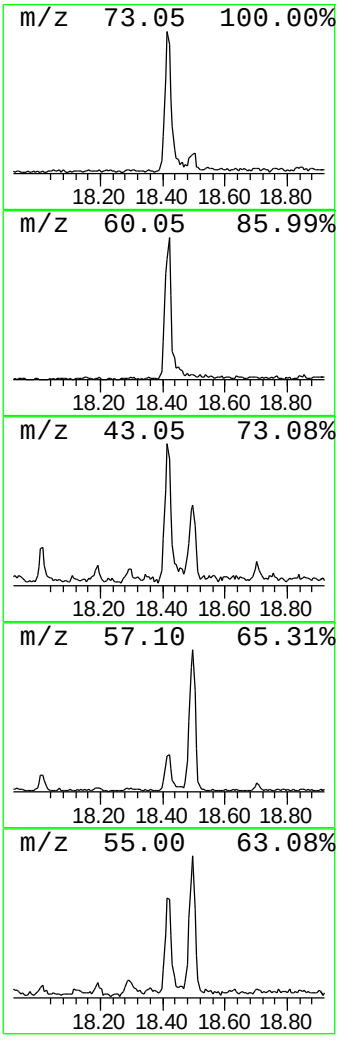
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	6.40 ng	746055	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023422.D
Acq On : 3 Aug 2016 12:19
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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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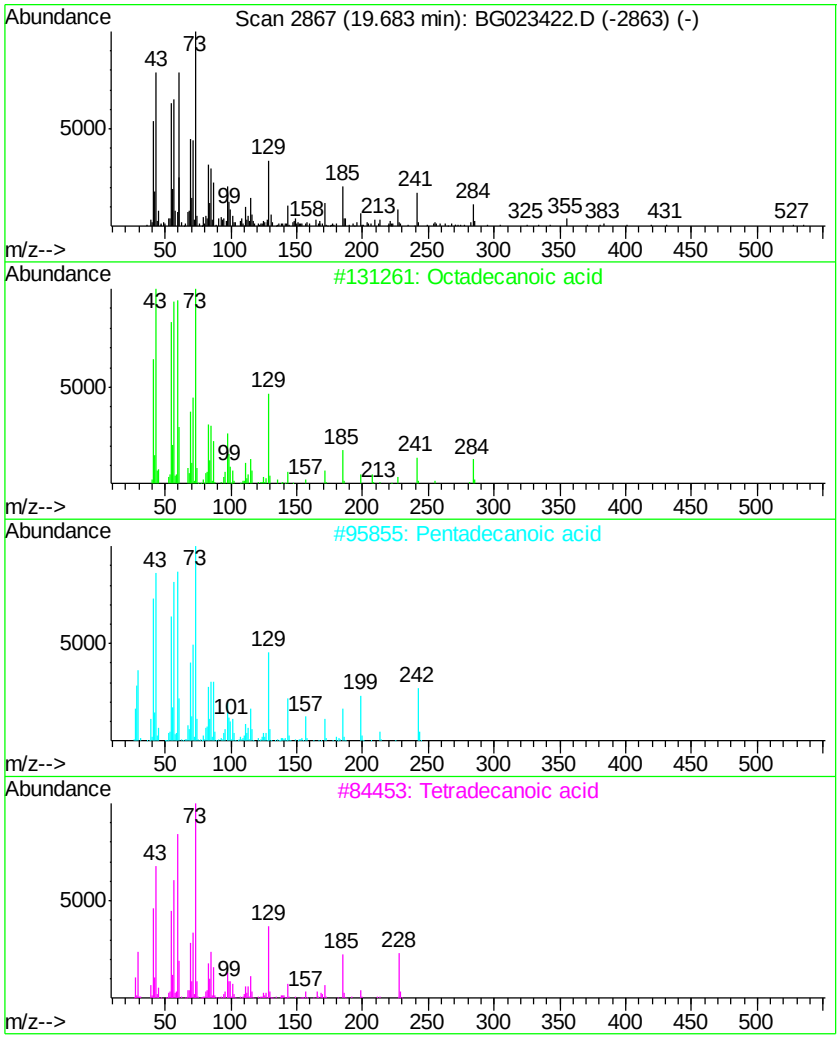
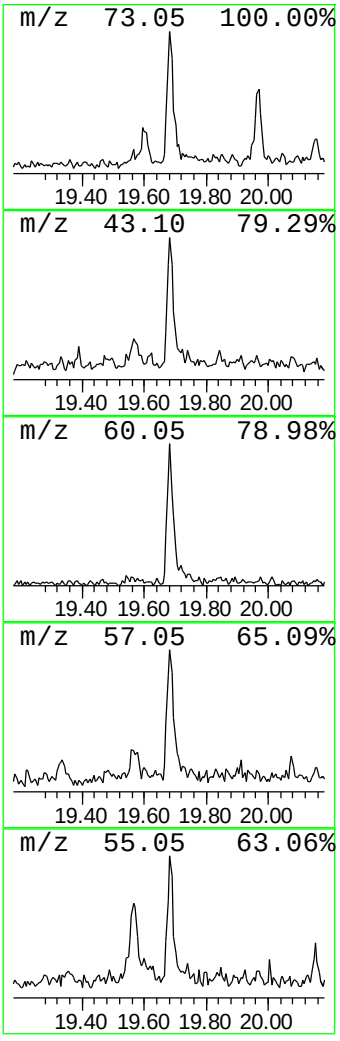
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	2.56 ng	297902	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74





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Misc :
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Instrument : BNA_G
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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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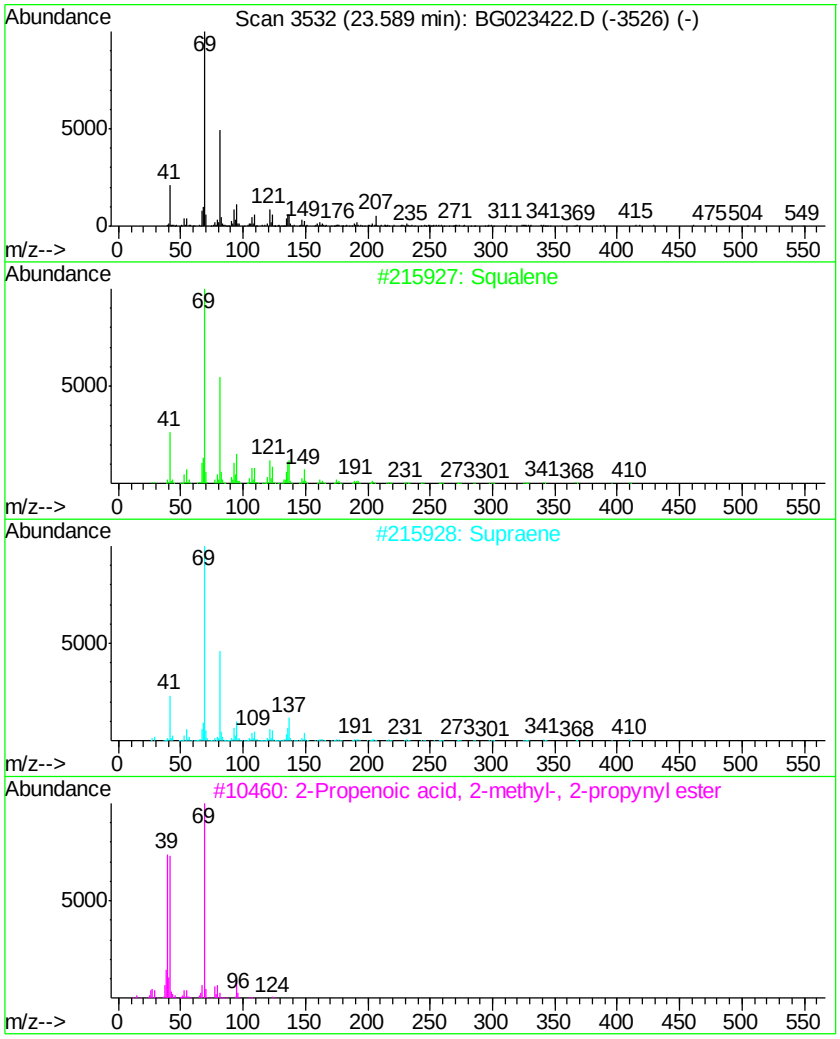
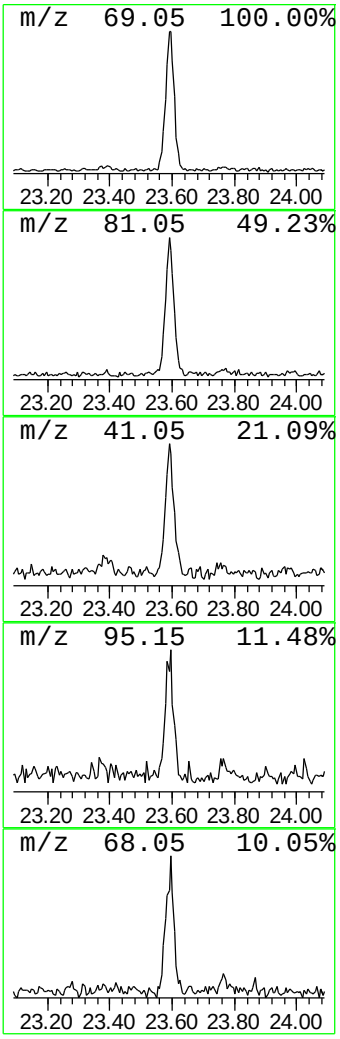
Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.59	3.95 ng	491554	Perylene-d12	25.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	72
2	Supraene	410	C30H50	007683-64-9	72
3	2-Propenoic acid, 2-methyl-, 2-p...	124	C7H8O2	013861-22-8	64
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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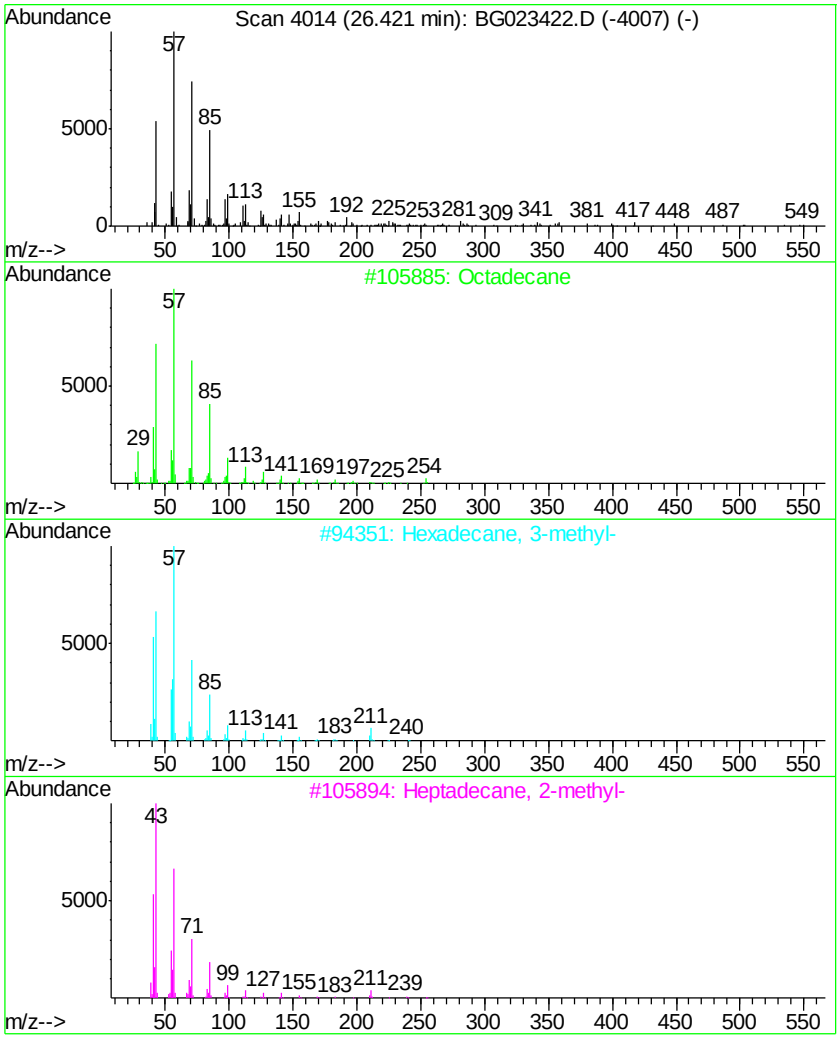
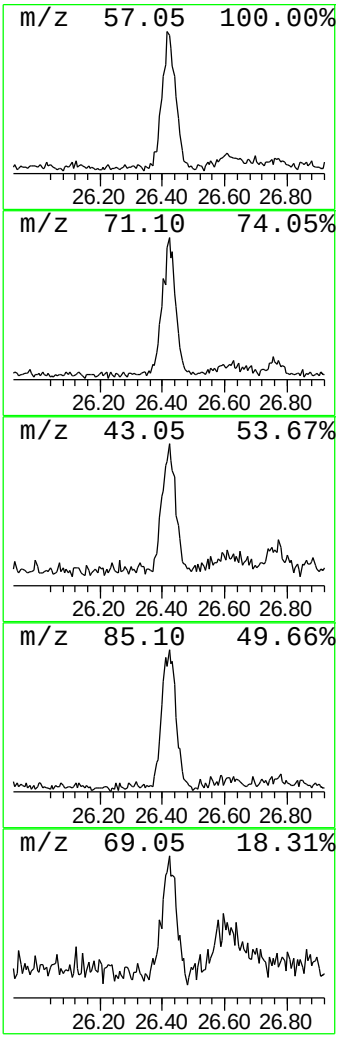
Peak Number 7 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.42	3.88 ng	482590	Perylene-d12	25.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	87
3	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
4	Hentriacontane	437	C31H64	000630-04-6	83
5	Dodecane	170	C12H26	000112-40-3	83





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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
Propane, 2,2-dime...	2.99	148.8	ng	4927920	1	8.13	662319	20.0
unknown5.18	5.18	7.8	ng	258720	1	8.13	662319	20.0
n-Hexadecanoic acid	18.42	6.4	ng	746055	4	17.54	2330990	20.0
Octadecanoic acid	19.68	2.6	ng	297902	4	17.54	2330990	20.0
Squalene	23.59	4.0	ng	491554	6	25.25	2486240	20.0
Octadecane	26.42	3.9	ng	482590	6	25.25	2486240	20.0