LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110218\
Data File : BG037770.D
Acq On : 3 Nov 2018 1:14
Operator : JU/SJ
Sample : J5803-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SODUS-TS-001

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	5.183	314	322	328	rBV	56850	98400	2.76%	0.415%
2	5.641	393	400	411	rVB	1125675	1837734	51.58%	7.758%
3	7.245	664	673	693	rBV	1240544	2341148	65.71%	9.883%
4	7.627	730	738	752	rBV	1129026	2028959	56.94%	8.565%
5	8.097	811	818	831	rVB	187698	340500	9.56%	1.437%
6	8.420	865	873	882	rBV	796470	1445121	40.56%	6.101%
7	9.278	1011	1019	1030	rBV	728749	1364039	38.28%	5.758%
8	10.923	1290	1299	1307	rBV	278148	530222	14.88%	2.238%
9	13.356	1705	1713	1725	rBV	1881170	3043150	85.41%	12.847%
10	14.178	1846	1853	1859	rBV	215396	333497	9.36%	1.408%
11	14.736	1940	1948	1956	rBV2	466618	797157	22.37%	3.365%
12	16.223	2193	2201	2210	rBV	1437002	2362702	66.31%	9.974%
13	17.480	2408	2415	2425	rBV	566665	912445	25.61%	3.852%
14	18.338	2554	2561	2571	rBV2	112453	202540	5.68%	0.855%
15	19.601	2772	2776	2782	rBV3	36006	60845	1.71%	0.257%
16	20.083	2851	2858	2866	rBV	2527897	3563106	100.00%	15.042%
17	21.387	3072	3080	3081	rBV4	44579	103336	2.90%	0.436%
18	21.763	3137	3144	3158	rBV	500811	928646	26.06%	3.920%
19	21.916	3166	3170	3175	rVB2	28897	42587	1.20%	0.180%
20	22.539	3271	3276	3281	rVB	35658	55842	1.57%	0.236%
21	23.244	3392	3396	3402	rVB3	25582	46790	1.31%	0.198%
22	23.450	3424	3431	3439	rVB	72353	147302	4.13%	0.622%
23	24.072	3531	3537	3548	rVB2	69960	161733	4.54%	0.683%
24	25.101	3698	3712	3727	rBV2	245021	845722	23.74%	3.570%
25	26.211	3894	3901	3911	rBV6	31045	94106	2.64%	0.397%

Sum of corrected areas: 23687629

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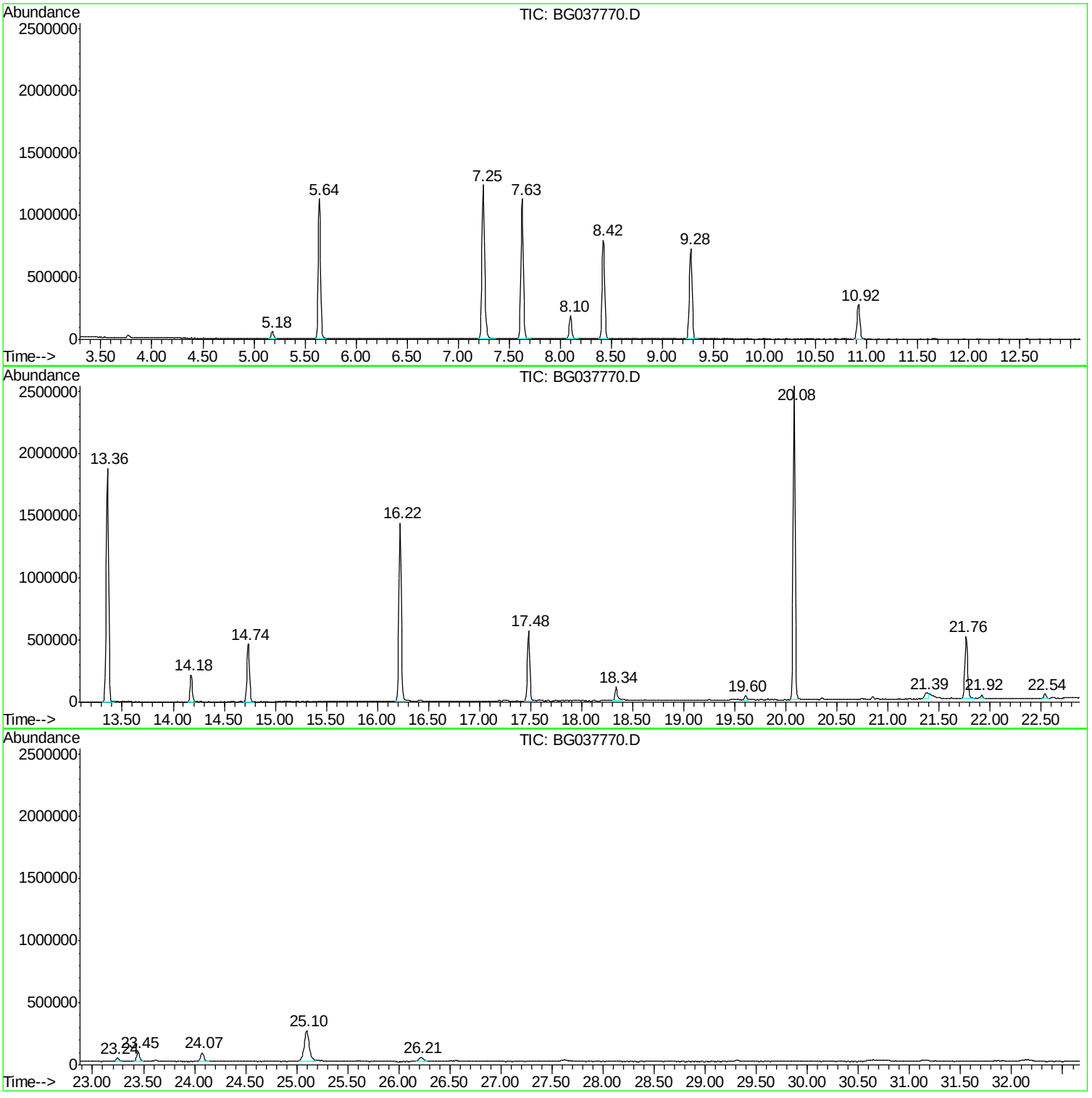
BNA_G
ClientSampleId :
SODUS-TS-001

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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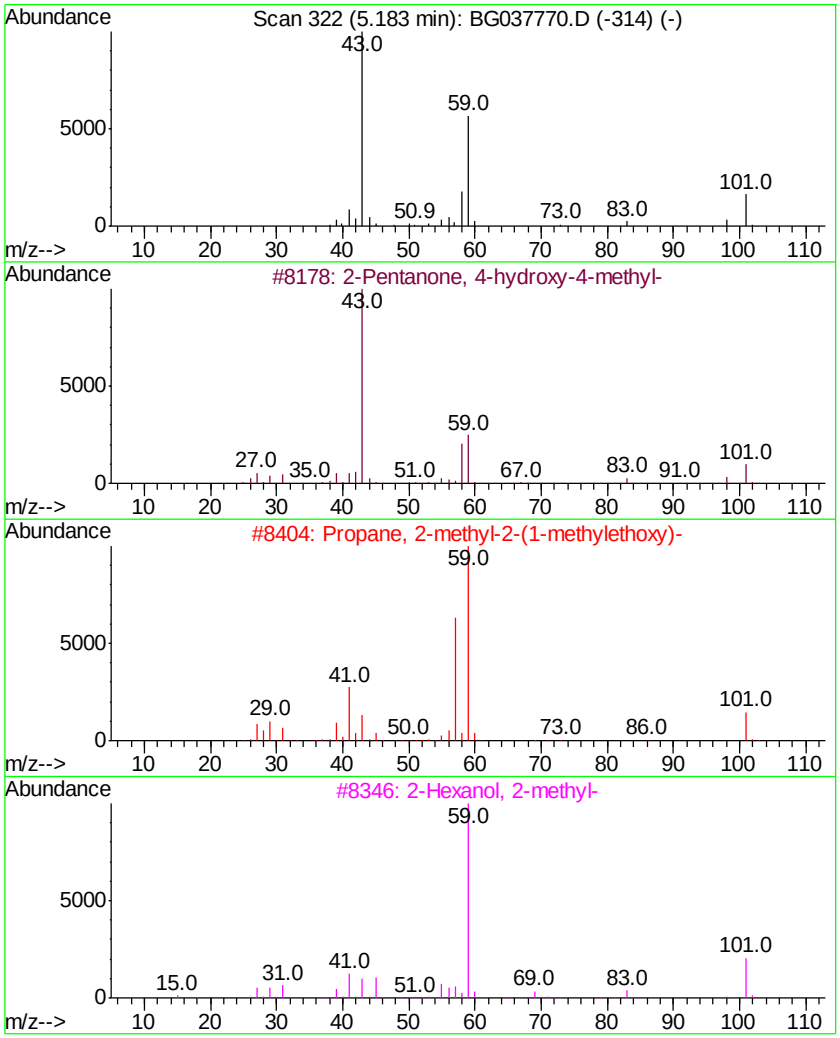
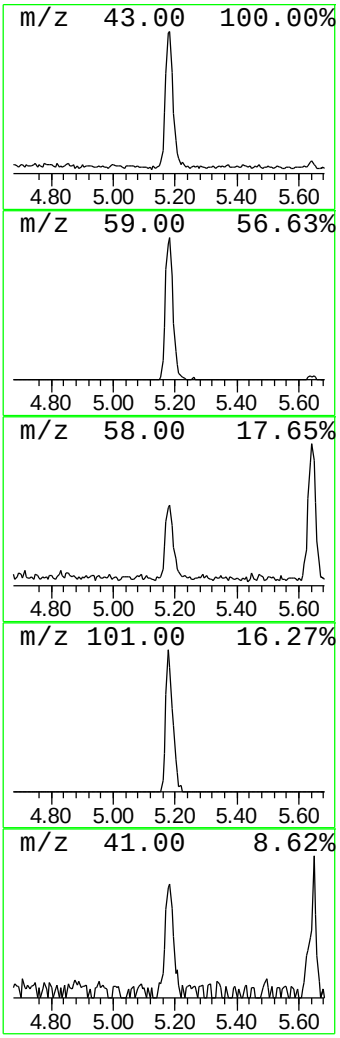
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	5.78 ng	98400	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SODUS-TS-001

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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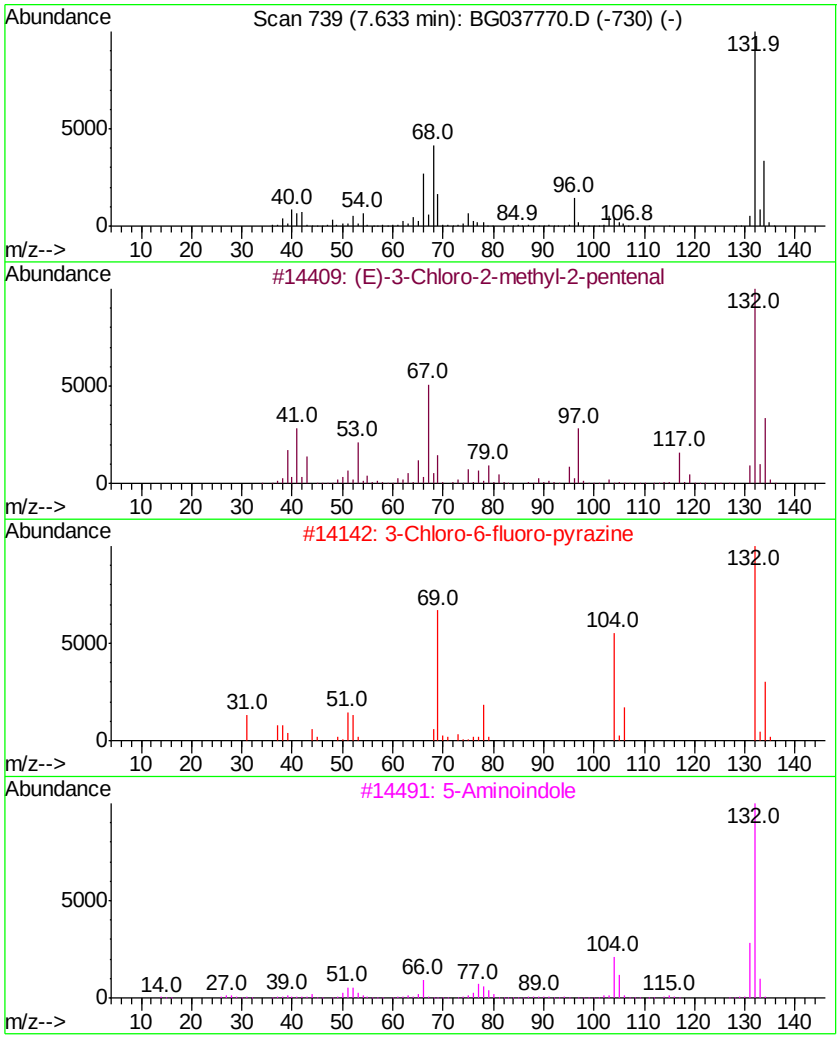
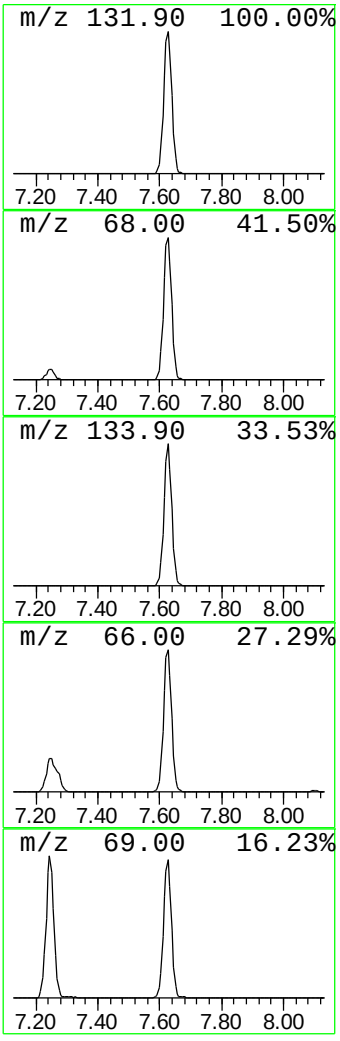
Peak Number 2 unknown7.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	119.18 ng	2028960	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Xenon	132	Xe	007440-63-3	9





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Acq On : 3 Nov 2018 1:14
Operator : JU/SJ
Sample : J5803-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SODUS-TS-001

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
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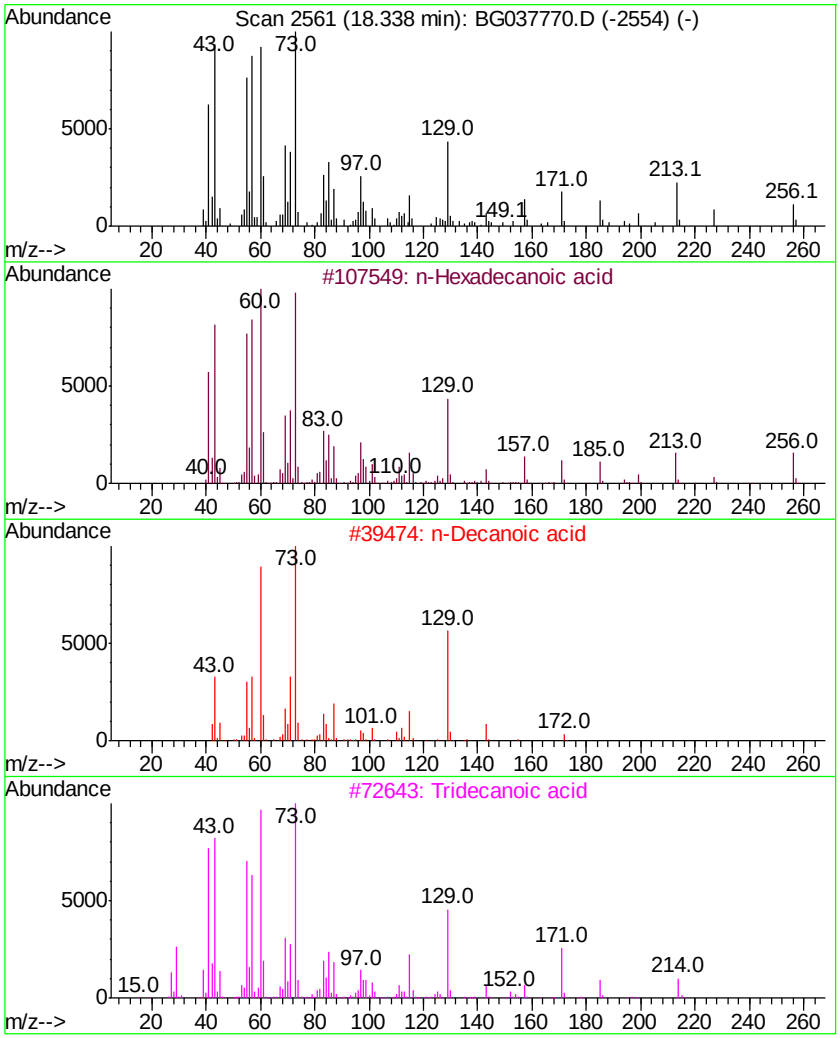
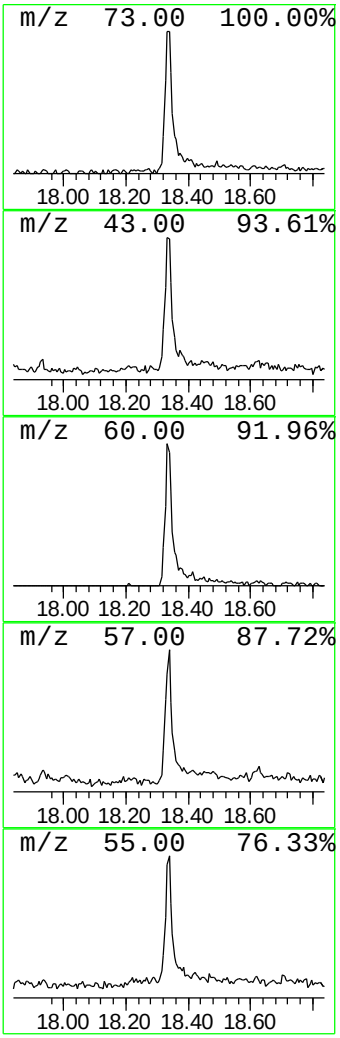
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	4.44 ng	202540	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Decanoic acid	172	C10H20O2	000334-48-5	92
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Acq On : 3 Nov 2018 1:14
Operator : JU/SJ
Sample : J5803-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SODUS-TS-001

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
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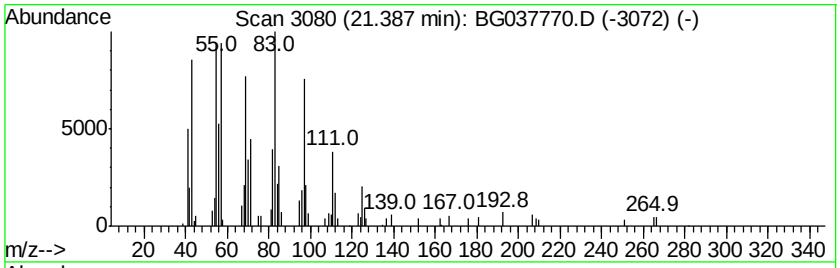
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

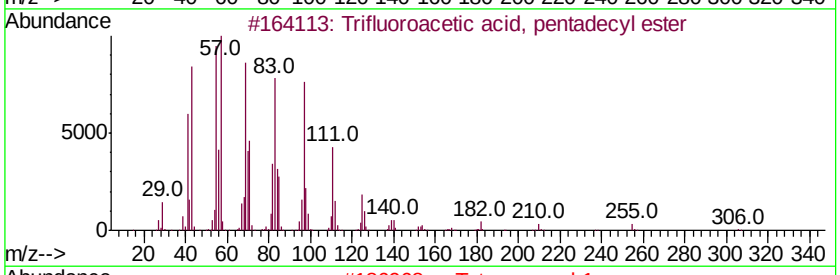
****

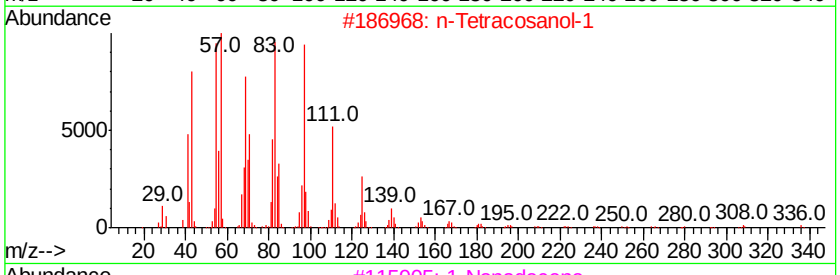
Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 7

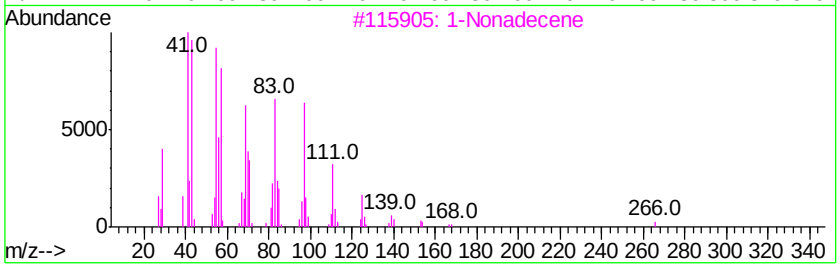
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.39	2.23 ng	103336	Chrysene-d12	21.76

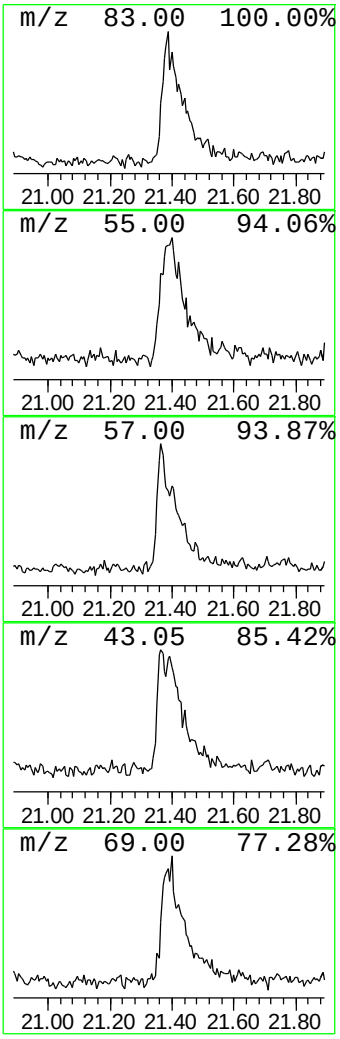
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Nonadecene	266	C19H38	018435-45-5	87
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87











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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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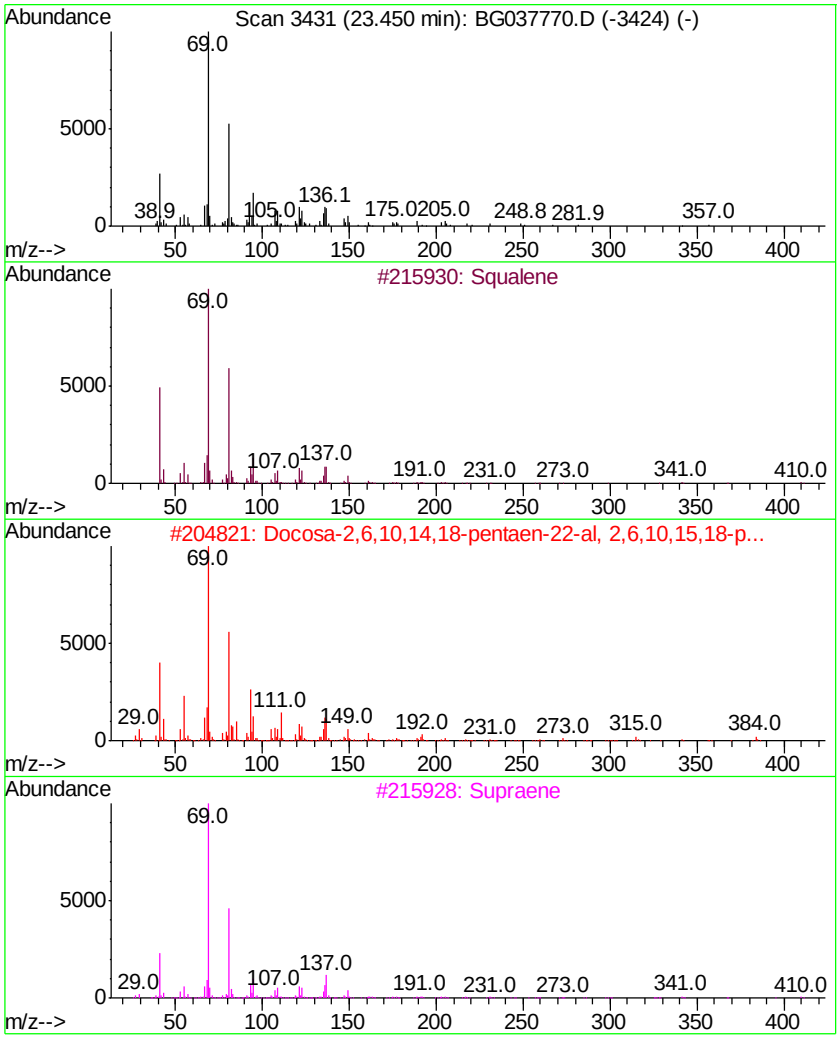
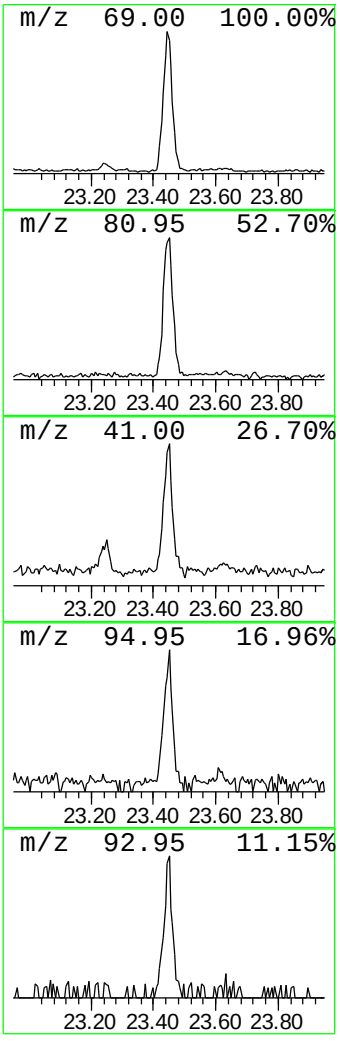
Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.45	3.48 ng	147302	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
3	Supraene	410	C30H50	007683-64-9	80
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64





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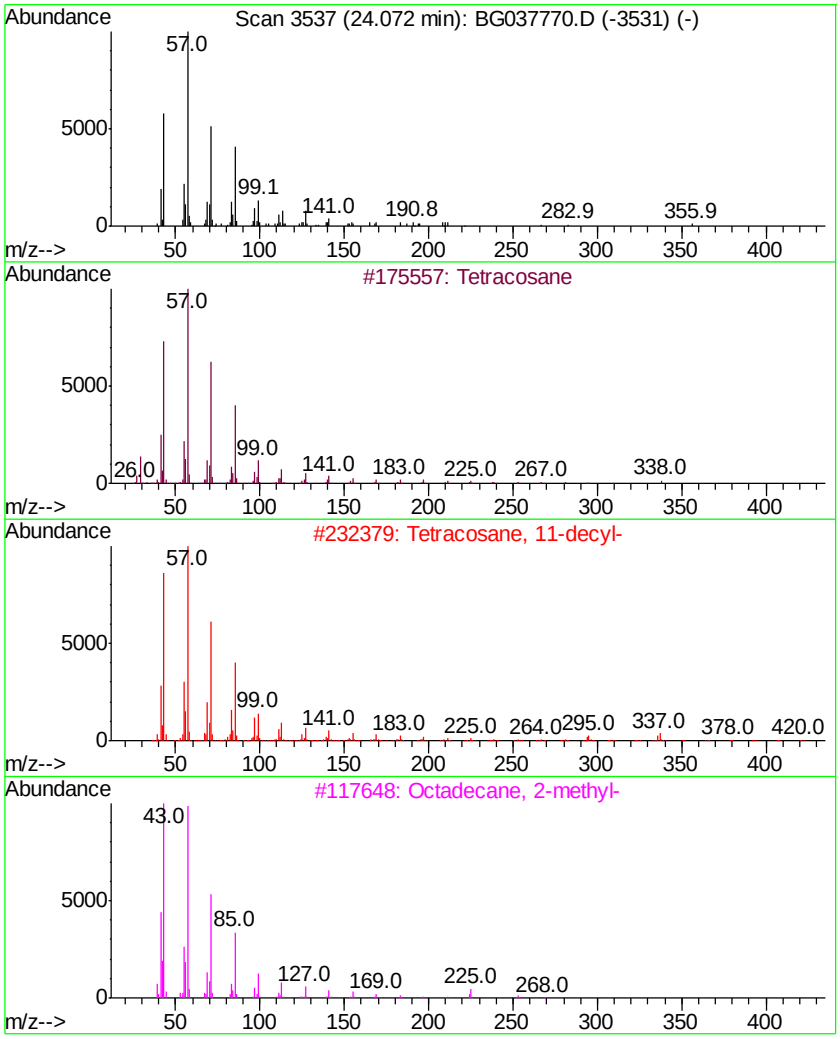
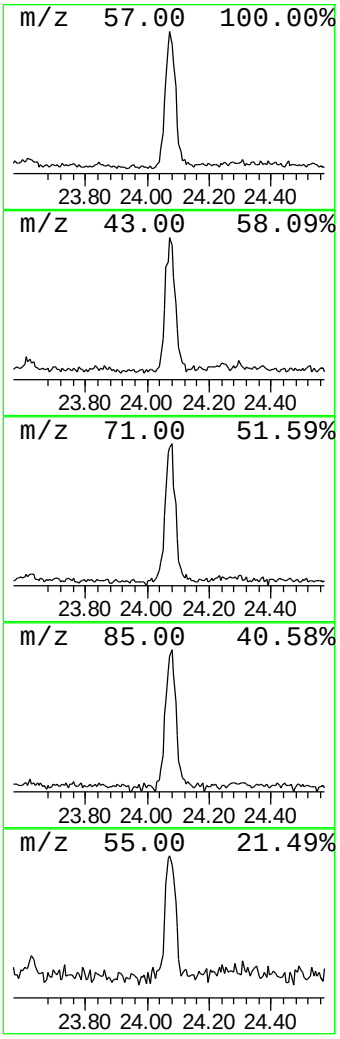
Peak Number 7 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.07	3.82 ng	161733	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	86
5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	83





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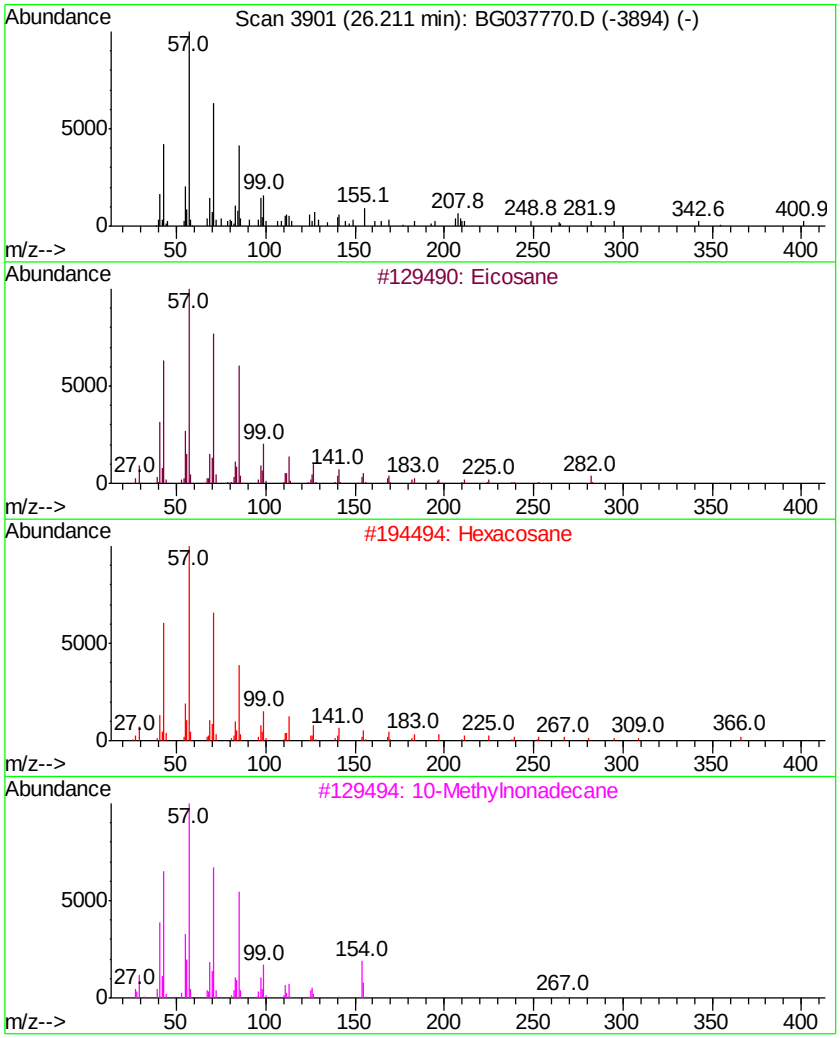
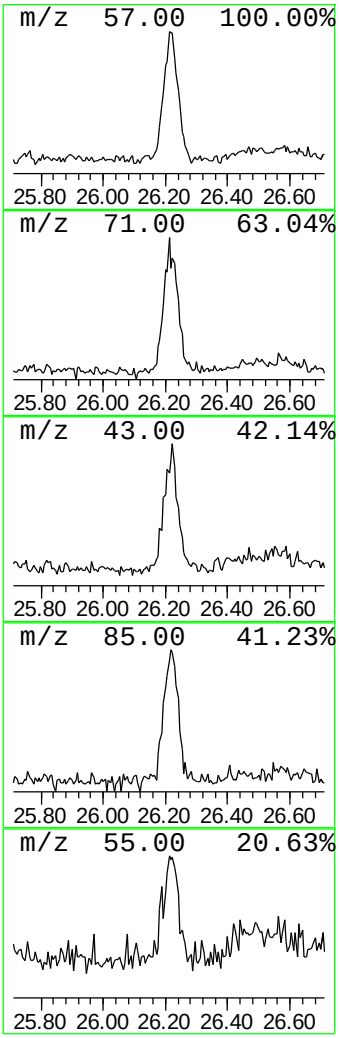
Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.21	2.23 ng	94106	Perylene-d12	25.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hexacosane	366	C26H54	000630-01-3	86
3	10-Methylnonadecane	282	C20H42	056862-62-5	86
4	Pentacosane	352	C25H52	000629-99-2	83
5	Hentriacontane	437	C31H64	000630-04-6	83





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	5.8	ng	98400	1	8.10	340500	20.0
unknown7.63	7.63	119.2	ng	2028960	1	8.10	340500	20.0
n-Hexadecanoic acid	18.34	4.4	ng	202540	4	17.48	912445	20.0
Trifluoroacetic a...	21.39	2.2	ng	103336	5	21.76	928646	20.0
Squalene	23.45	3.5	ng	147302	6	25.10	845722	20.0
Tetracosane	24.07	3.8	ng	161733	6	25.10	845722	20.0
Eicosane	26.21	2.2	ng	94106	6	25.10	845722	20.0