LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050515.D
Acq On : 8 Oct 2021 18:57
Operator : CG/JU
Sample : M4117-02
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument : BNA_G
ClientSampleId : SB-1(3-3.5)

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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050515.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.333	307	314	321	rBV	65243	106108	4.86%	0.670%
2	5.797	386	393	406	rBV	647489	1079323	49.45%	6.815%
3	7.401	658	666	677	rBV	670875	1190487	54.55%	7.517%
4	8.259	804	812	825	rBV	298937	535665	24.54%	3.382%
5	9.428	999	1011	1022	rBV	416216	786808	36.05%	4.968%
6	10.832	1243	1250	1261	rVB	55872	102464	4.69%	0.647%
7	11.085	1281	1293	1301	rBV	400576	744576	34.11%	4.702%
8	13.500	1697	1704	1712	rBV	941325	1501901	68.81%	9.484%
9	14.880	1932	1939	1947	rVB	602266	980812	44.94%	6.193%
10	16.355	2184	2190	2200	rVB	679341	1068547	48.96%	6.747%
11	17.618	2399	2405	2412	rVB	738754	1175869	53.88%	7.425%
12	18.006	2467	2471	2472	rBV2	29705	35652	1.63%	0.225%
13	18.182	2490	2501	2512	rBV	225491	895626	41.04%	5.655%
14	18.476	2548	2551	2558	rVB4	29074	46597	2.13%	0.294%
15	19.416	2708	2711	2715	rBV4	26728	27888	1.28%	0.176%
16	20.086	2821	2825	2831	rVB2	42040	74354	3.41%	0.470%
17	20.209	2840	2846	2852	rVB	1684865	2182553	100.00%	13.782%
18	20.879	2955	2960	2967	rVB2	68798	138595	6.35%	0.875%
19	21.520	3064	3069	3075	rBV	79075	128432	5.88%	0.811%
20	21.749	3102	3108	3116	rVB2	92331	209841	9.61%	1.325%
21	21.919	3130	3137	3145	rVB2	711898	1239198	56.78%	7.825%
22	22.747	3271	3278	3290	rVB	98213	280735	12.86%	1.773%
23	25.339	3709	3719	3729	rBV2	419726	1304474	59.77%	8.237%

Sum of corrected areas: 15836505

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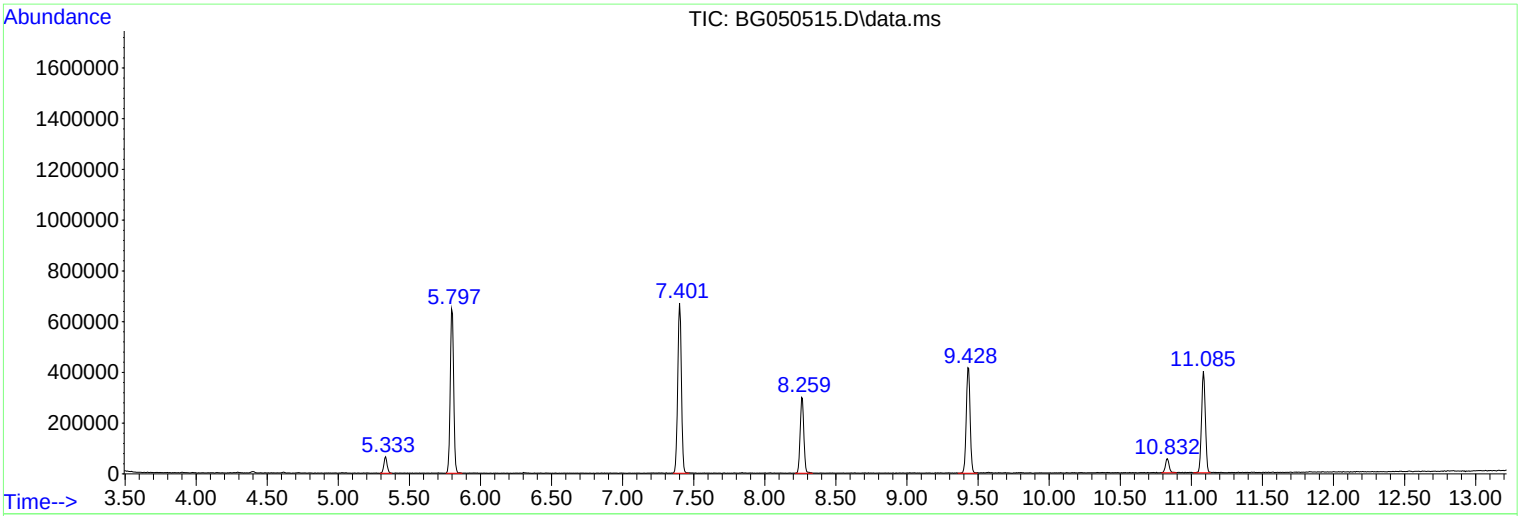
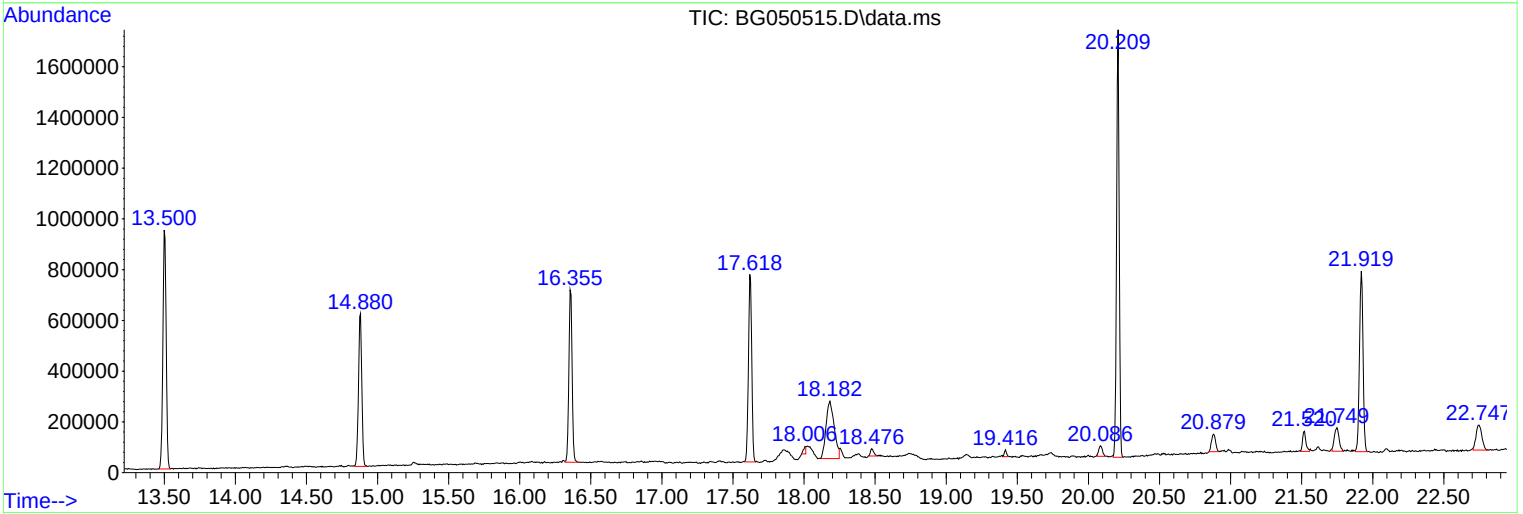
Misc :
ALS Vial : 4 Sample Multiplier: 2

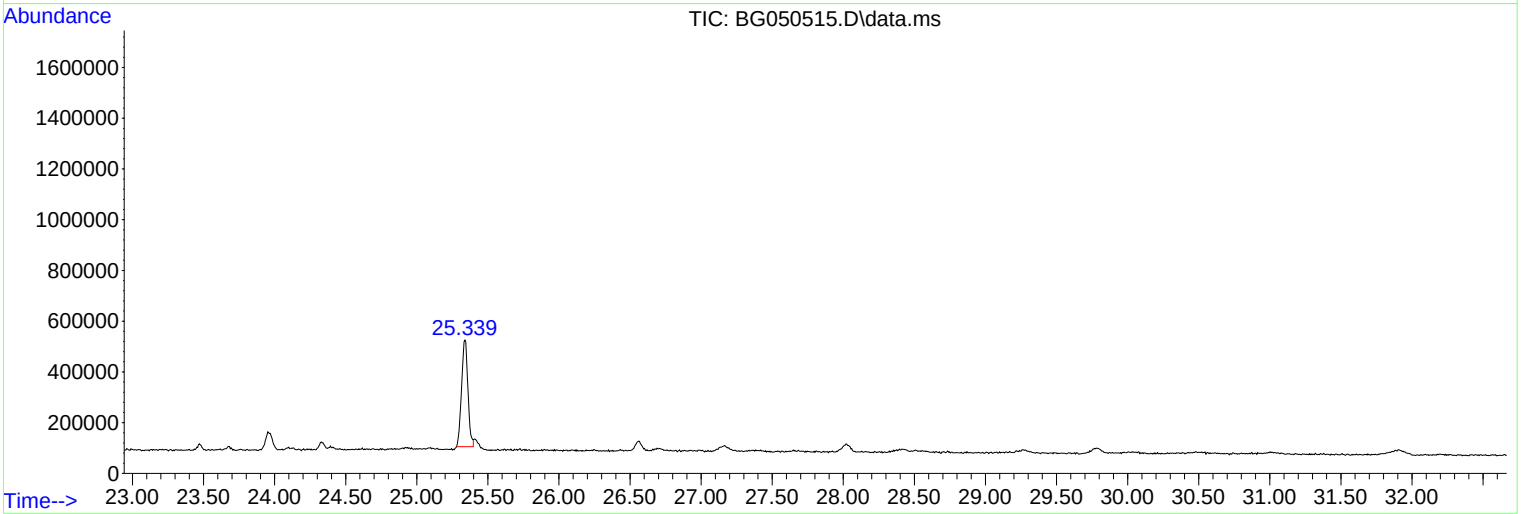
Instrument :
BNA_G
ClientSampleId :
SB-1(3-3.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BG050515.D
Acq On : 8 Oct 2021 18:57
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Sample : M4117-02
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Instrument : BNA_G
ClientSampleId : SB-1(3-3.5)

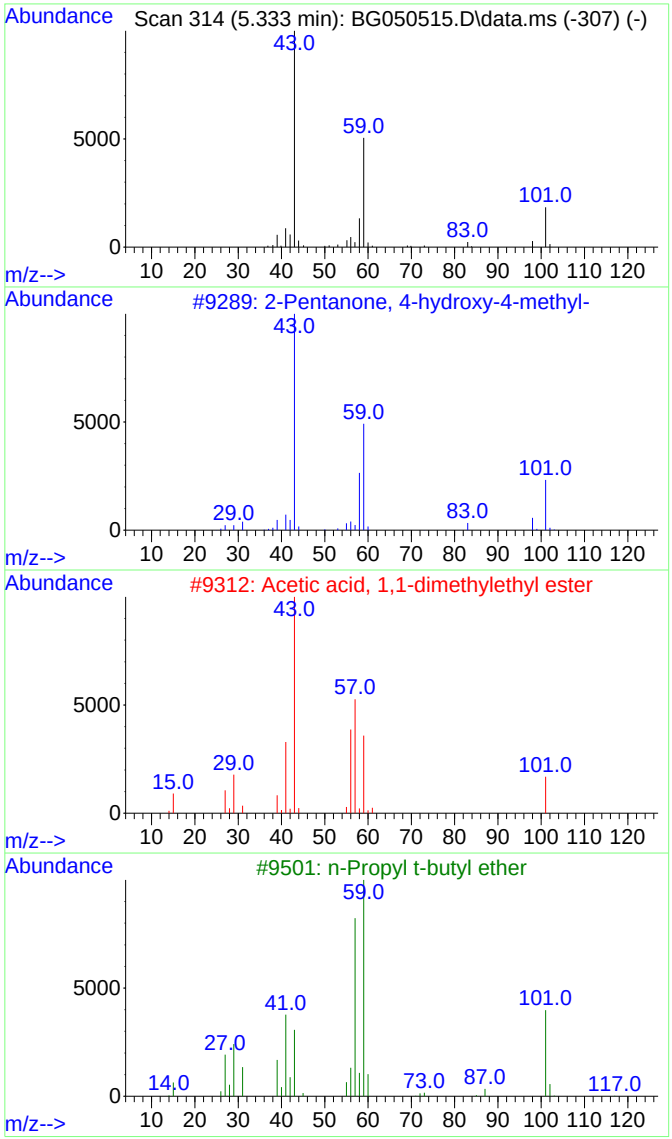
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

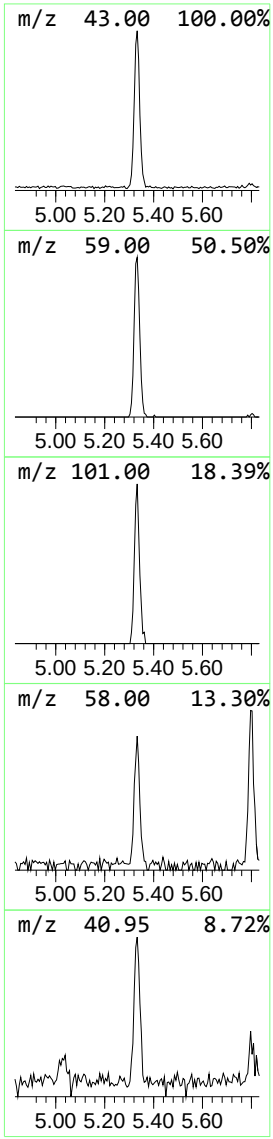
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.333	3.96 ng	106108	1,4-Dichlorobenzene-d4	8.264

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	25
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23





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Operator : CG/JU
Sample : M4117-02
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument : BNA_G
ClientSampleId : SB-1(3-3.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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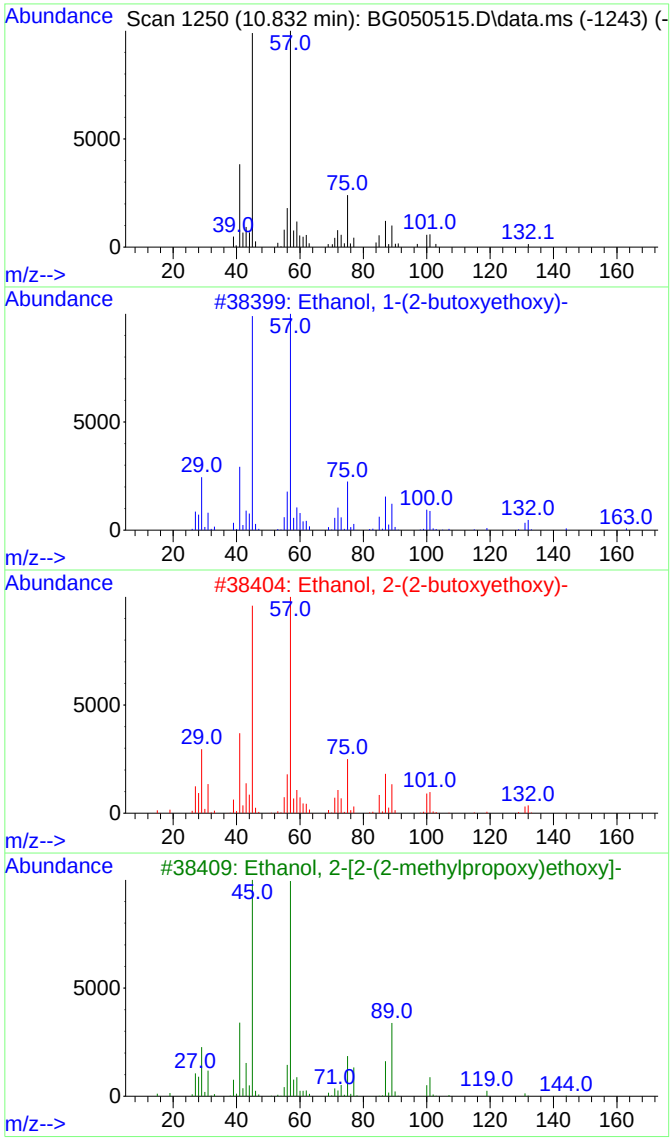
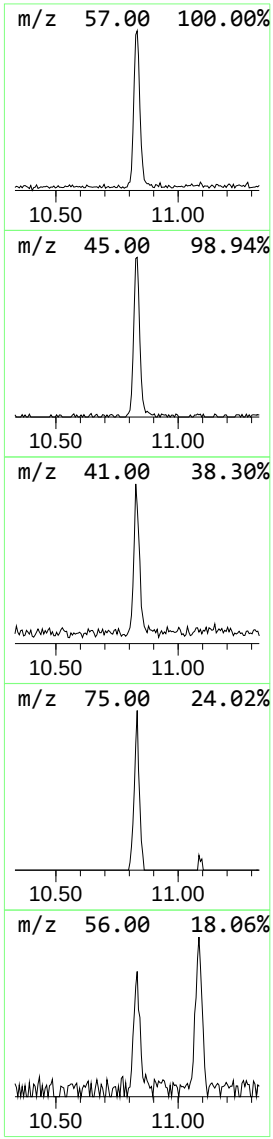
****

Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.832	2.75 ng	102464	Naphthalene-d8	11.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050515.D
Acq On : 8 Oct 2021 18:57
Operator : CG/JU
Sample : M4117-02
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument :
BNA_G
ClientSampleId :
SB-1(3-3.5)

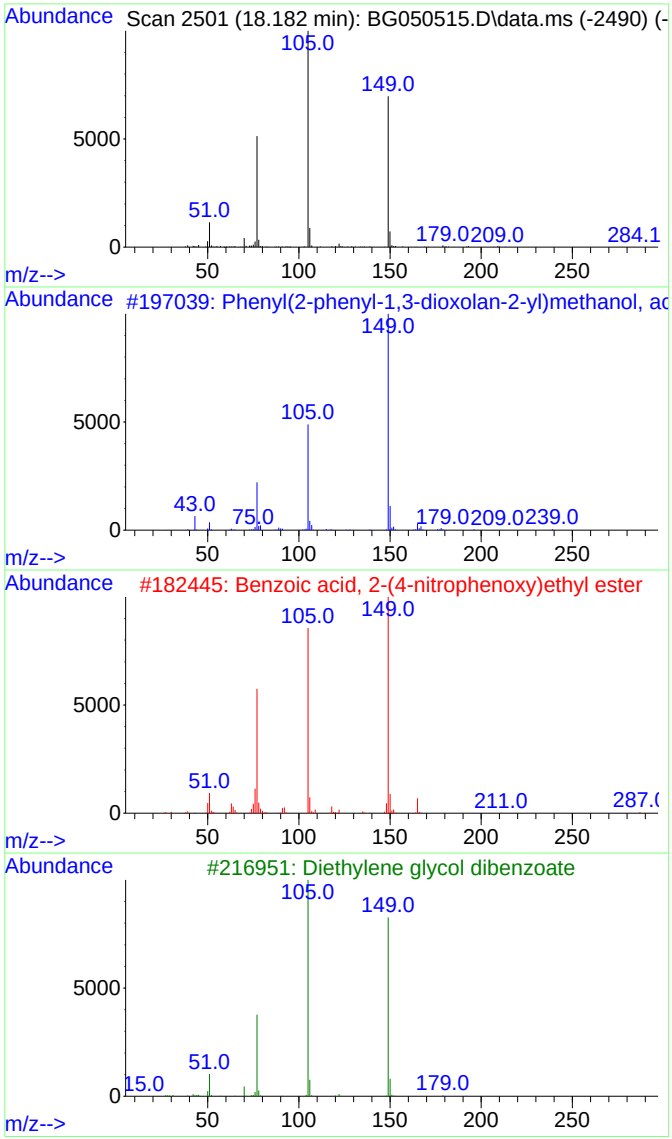
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

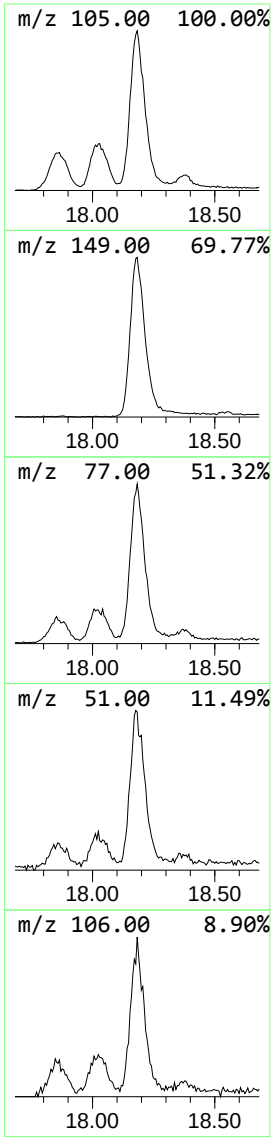
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenyl(2-phenyl-1,3-dioxola... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.182	15.23 ng	895626	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	78
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
5	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	59





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Operator : CG/JU
Sample : M4117-02
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument : BNA_G
ClientSampleId : SB-1(3-3.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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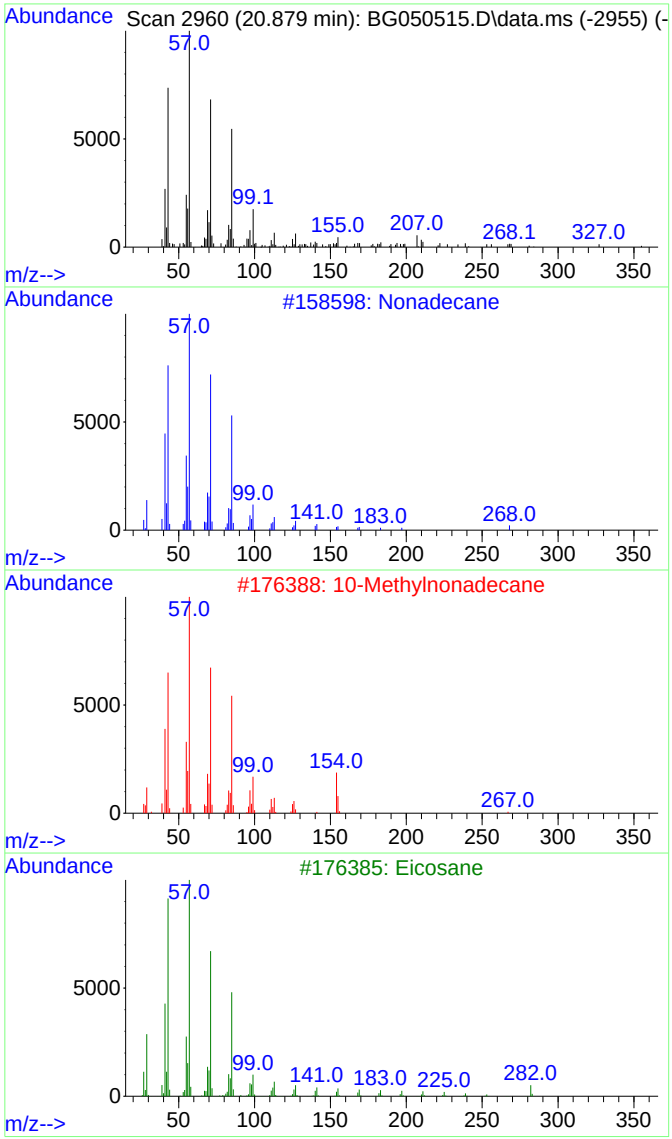
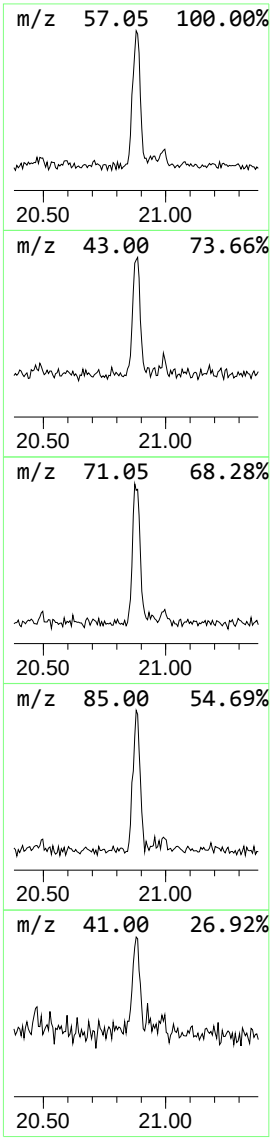
****

Peak Number 4 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.879	2.24 ng	138595	Chrysene-d12	21.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	10-Methylnonadecane	282	C20H42	056862-62-5	83
3	Eicosane	282	C20H42	000112-95-8	83
4	Pentadecane	212	C15H32	000629-62-9	80
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	80





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Data File : BG050515.D
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Operator : CG/JU
Sample : M4117-02
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument : BNA_G
ClientSampleId : SB-1(3-3.5)

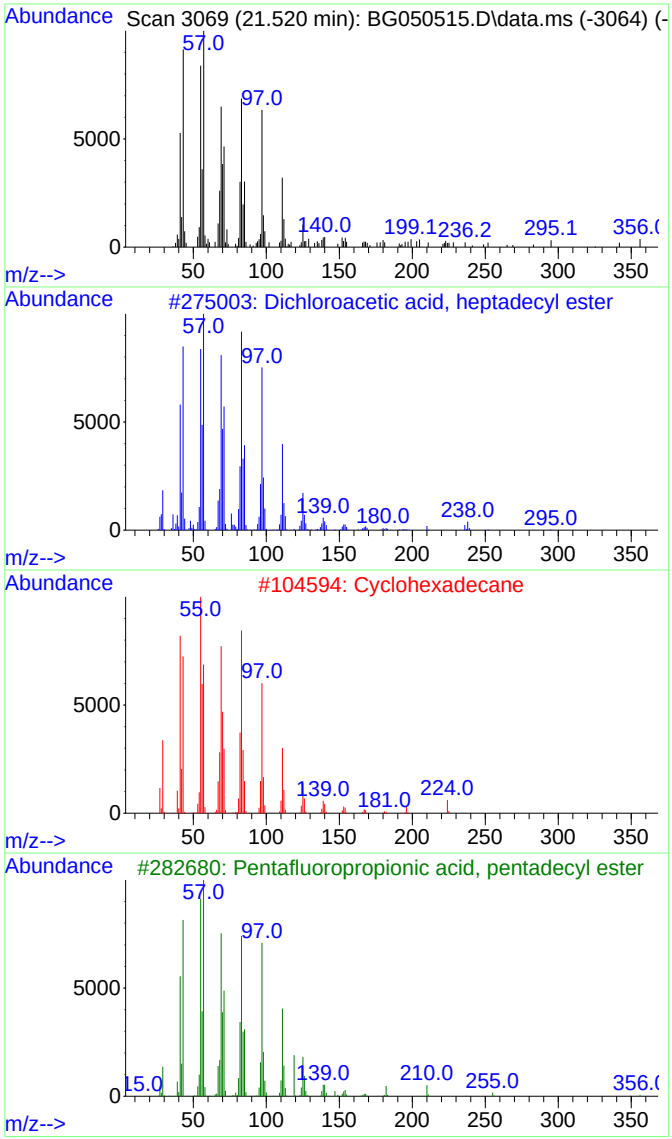
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

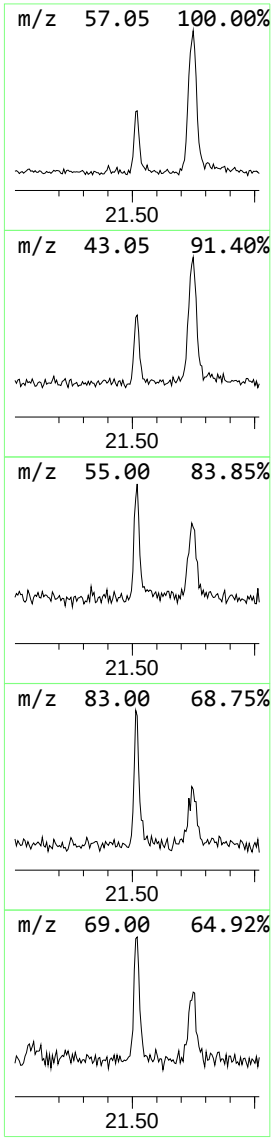
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.520	2.07 ng	128432	Chrysene-d12	21.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2	Cyclohexadecane	224	C16H32	000295-65-8	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





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Sample : M4117-02
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument : BNA_G
ClientSampleId : SB-1(3-3.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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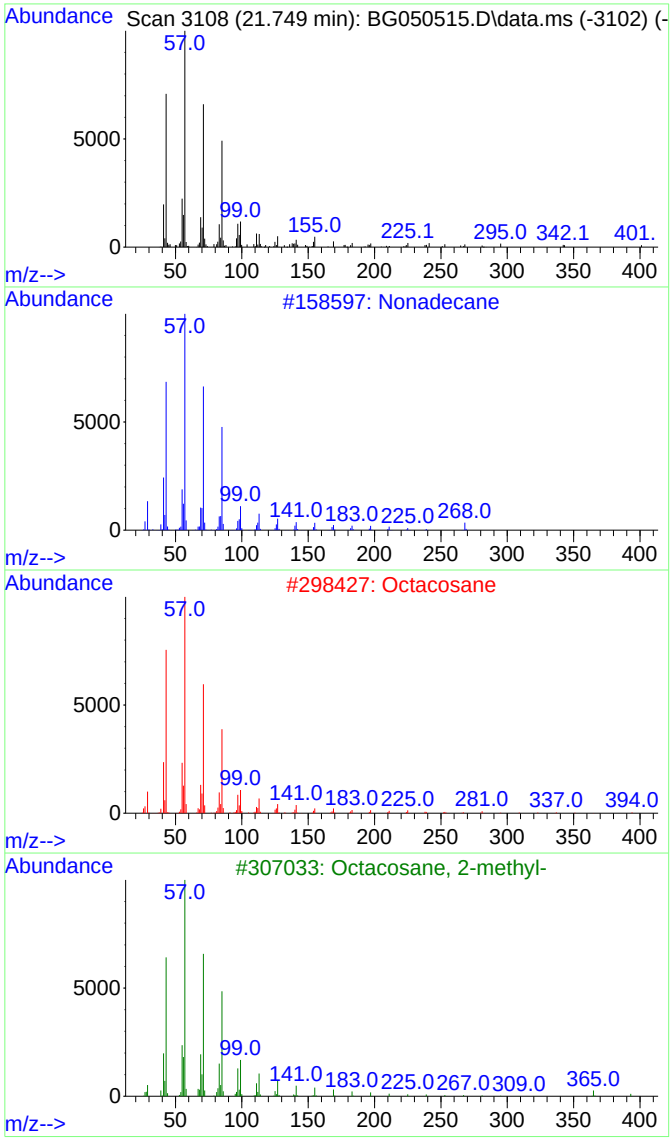
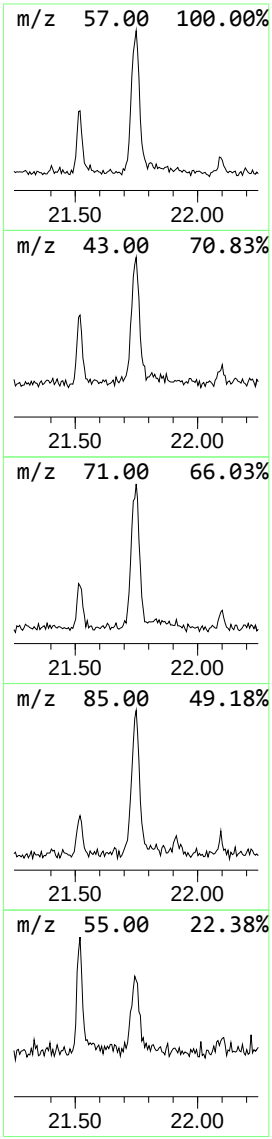
****

Peak Number 6 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.749	3.39 ng	209841	Chrysene-d12	21.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Octacosane	394	C28H58	000630-02-4	90
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4	Decane, 1-iodo-	268	C10H21I	002050-77-3	87
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83





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Sample : M4117-02
Misc :
ALS Vial : 4 Sample Multiplier: 2

Instrument : BNA_G
ClientSampleId : SB-1(3-3.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

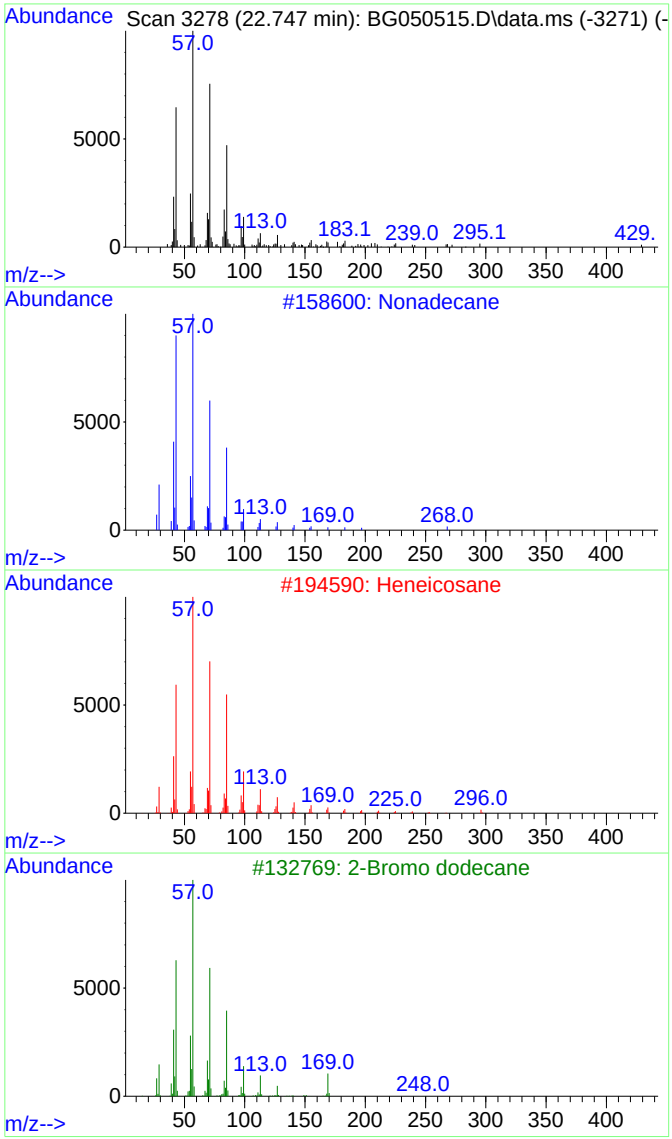
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

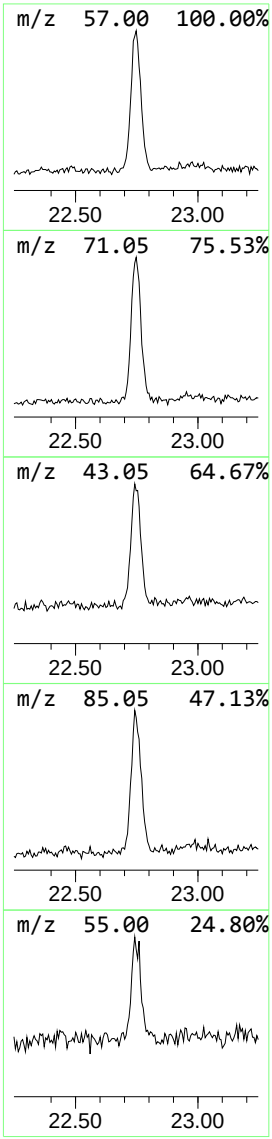
****

Peak Number 7 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.747	4.53 ng	280735	Chrysene-d12	21.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
4	Tetradecane	198	C14H30	000629-59-4	80
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.333	4.0	ng	106108	1	8.264	535665	20.0
Ethanol, 1-(2-b...	10.832	2.8	ng	102464	2	11.085	744576	20.0
Phenyl(2-phenyl...	18.182	15.2	ng	895626	4	17.618	1175870	20.0
Nonadecane	20.879	2.2	ng	138595	5	21.919	1239200	20.0
Dichloroacetic ...	21.520	2.1	ng	128432	5	21.919	1239200	20.0
Octacosane	21.749	3.4	ng	209841	5	21.919	1239200	20.0
Heneicosane	22.747	4.5	ng	280735	5	21.919	1239200	20.0