LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-41114-15

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-BG021021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048329.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.666	50	56	65	rVB	29655	51469	1.47%	0.200%
2	3.854	84	88	99	rVB2	32306	55911	1.59%	0.217%
3	4.953	269	275	281	rBV	35880	54483	1.55%	0.212%
4	5.188	309	315	322	rVB3	22029	46168	1.32%	0.179%
5	5.693	377	401	416	rBV	512591	1123453	32.04%	4.367%
6	6.175	473	483	498	rBV	1187721	2070379	59.04%	8.047%
7	6.504	532	539	548	rVB	27229	52329	1.49%	0.203%
8	6.727	570	577	584	rBV	129396	223478	6.37%	0.869%
9	7.156	640	650	654	rBV3	50317	119481	3.41%	0.464%
10	7.315	669	677	690	rBV2	284565	629131	17.94%	2.445%
11	8.102	805	811	816	rBV	170768	291247	8.31%	1.132%
12	8.161	816	821	834	rVB	786088	1337471	38.14%	5.199%
13	8.360	846	855	870	rVV2	90370	240086	6.85%	0.933%
14	8.490	872	877	890	rVB3	21202	50617	1.44%	0.197%
15	8.789	909	928	940	rBV3	137709	578331	16.49%	2.248%
16	8.907	940	948	958	rVB7	56267	170451	4.86%	0.663%
17	9.283	1004	1012	1021	rBV	599064	1099052	31.34%	4.272%
18	9.541	1033	1056	1060	rBV	298869	1263430	36.03%	4.911%
19	9.612	1064	1068	1072	rVB2	43872	63464	1.81%	0.247%
20	9.823	1094	1104	1111	rBV2	142614	375058	10.70%	1.458%
21	10.258	1169	1178	1186	rBV5	47495	168000	4.79%	0.653%
22	10.687	1243	1251	1259	rBV4	64422	163856	4.67%	0.637%
23	10.922	1283	1291	1298	rBV	204974	398420	11.36%	1.549%
24	11.081	1312	1318	1330	rVB5	20542	58945	1.68%	0.229%
25	11.586	1398	1404	1411	rVB2	52375	103342	2.95%	0.402%
26	11.757	1426	1433	1434	rBV5	24711	41537	1.18%	0.161%
27	11.898	1450	1457	1469	rVB5	30253	109631	3.13%	0.426%
28	12.567	1567	1571	1578	rBV4	20595	41589	1.19%	0.162%
29	12.702	1586	1594	1600	rBV4	44110	114659	3.27%	0.446%
30	13.090	1656	1660	1666	rVB3	24658	41199	1.17%	0.160%
31	13.190	1670	1677	1685	rBV7	47767	136449	3.89%	0.530%
32	13.361	1696	1706	1712	rVB	1504198	2388416	68.11%	9.284%
33	13.531	1729	1735	1740	rBV8	19591	42045	1.20%	0.163%
34	13.619	1744	1750	1755	rVB5	25350	56810	1.62%	0.221%
35	13.754	1769	1773	1784	rVB9	21964	46282	1.32%	0.180%
36	14.071	1821	1827	1838	rVB	88799	167213	4.77%	0.650%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-41114-15

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-BG021021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.183	1843	1846	1854	rVB3	25070	51407	1.47%	0.200%
38	14.265	1854	1860	1870	rBV	281148	567353	16.18%	2.205%
39	14.371	1874	1878	1884	rVB6	48681	82301	2.35%	0.320%
40	14.735	1934	1940	1948	rVB2	351654	582755	16.62%	2.265%
41	15.470	2061	2065	2070	rBV2	32748	50324	1.44%	0.196%
42	15.540	2075	2077	2084	rVB3	28665	45075	1.29%	0.175%
43	15.875	2129	2134	2138	rBV	58765	102135	2.91%	0.397%
44	15.928	2138	2143	2156	rVB	367426	634081	18.08%	2.465%
45	16.234	2188	2195	2201	rBV	1348359	2054836	58.60%	7.987%
46	16.792	2286	2290	2301	rVB	137451	241713	6.89%	0.940%
47	17.485	2402	2408	2414	rBV	443986	649891	18.53%	2.526%
48	17.585	2421	2425	2430	rBV5	29602	57935	1.65%	0.225%
49	17.667	2436	2439	2446	rBV5	36637	53682	1.53%	0.209%
50	17.879	2472	2475	2479	rVB3	37341	45059	1.28%	0.175%
51	18.384	2554	2561	2566	rBV3	72980	161228	4.60%	0.627%
52	18.801	2628	2632	2634	rBV3	38838	57379	1.64%	0.223%
53	18.836	2634	2638	2655	rVB3	458294	774692	22.09%	3.011%
54	19.101	2679	2683	2687	rBV	167075	224147	6.39%	0.871%
55	19.189	2695	2698	2706	rVB	48434	68857	1.96%	0.268%
56	19.259	2706	2710	2711	rVV3	32057	39122	1.12%	0.152%
57	19.289	2713	2715	2721	rVB3	61137	77947	2.22%	0.303%
58	19.730	2788	2790	2795	rVB2	31910	38150	1.09%	0.148%
59	20.082	2844	2850	2856	rBV	2716722	3506775	100.00%	13.630%
60	20.887	2984	2987	2993	rVB2	47906	67103	1.91%	0.261%
61	21.187	3035	3038	3042	rBV	36555	48406	1.38%	0.188%
62	21.762	3131	3136	3146	rVB	436885	751742	21.44%	2.922%
63	25.059	3689	3697	3707	rVB2	239144	719448	20.52%	2.796%

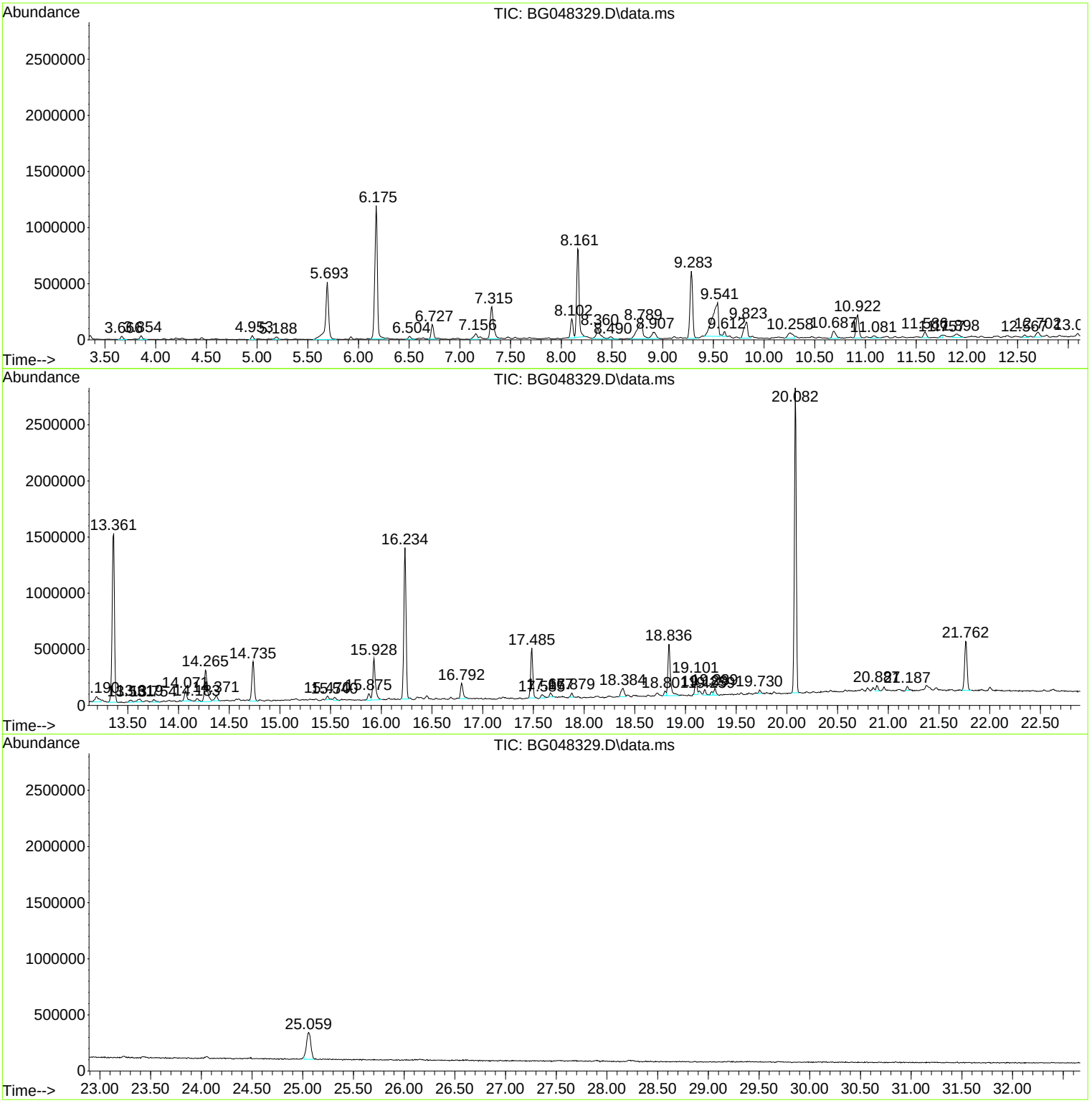
Sum of corrected areas: 25727425

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-41114-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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Data File : BG048329.D
Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

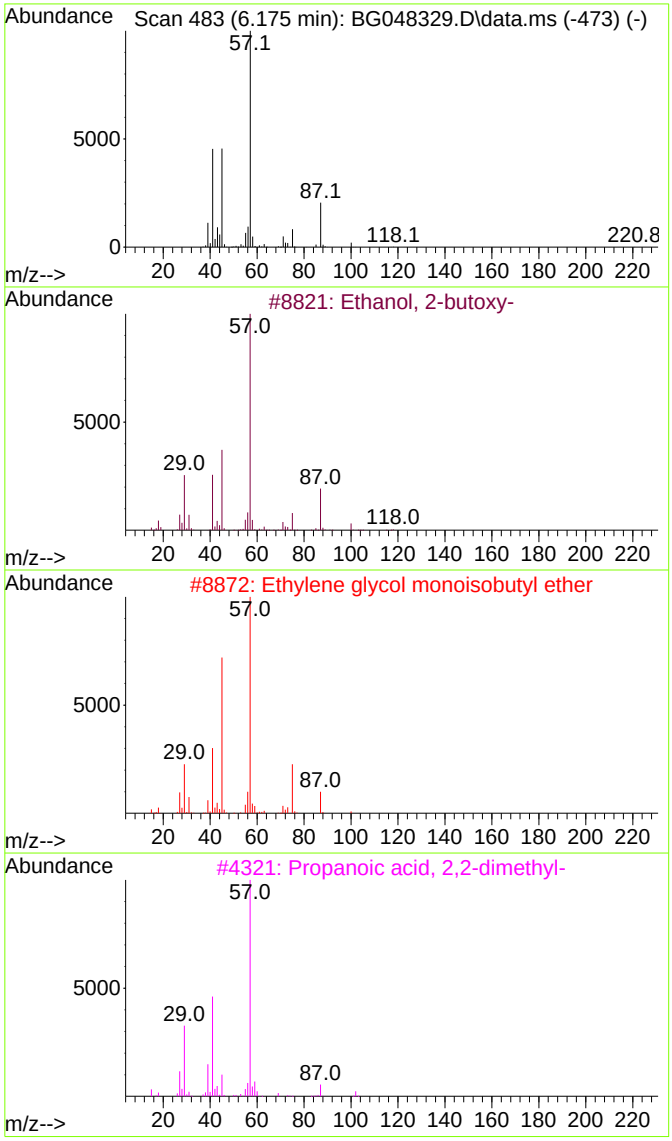
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

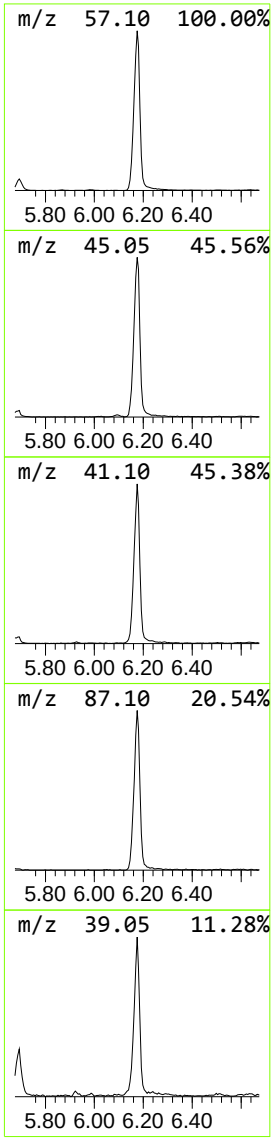
****

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.175	142.17 ng	2070380	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	64
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
3	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	25
4	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	23
5	n-Butyl ether	130	C8H18O	000142-96-1	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-41114-15

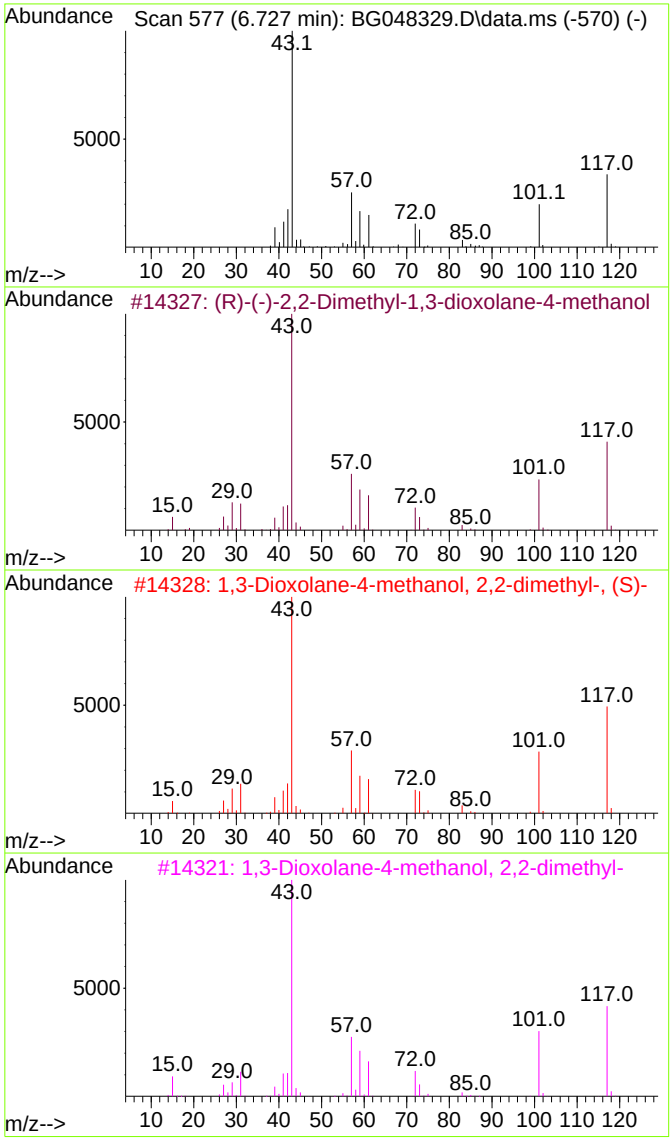
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

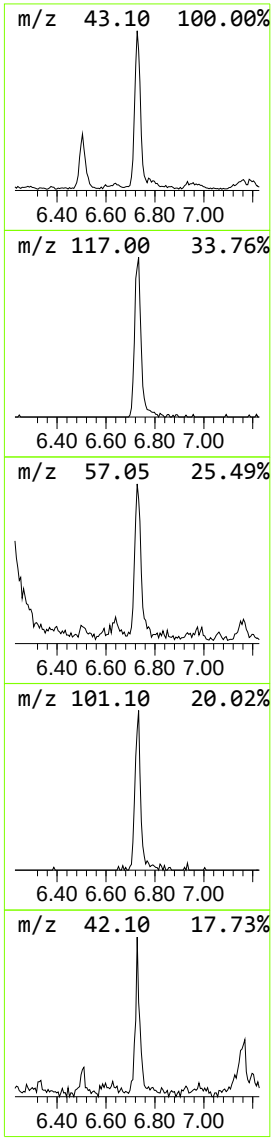
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (R)-(-)-2,2-Dimethyl-1,3-di... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.727	15.35 ng	223478	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(-)-2,2-Dimethyl-1,3-dioxola...	132	C6H12O3	014347-78-5	90
2	1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	022323-82-6	90
3	1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	000100-79-8	72
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-41114-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

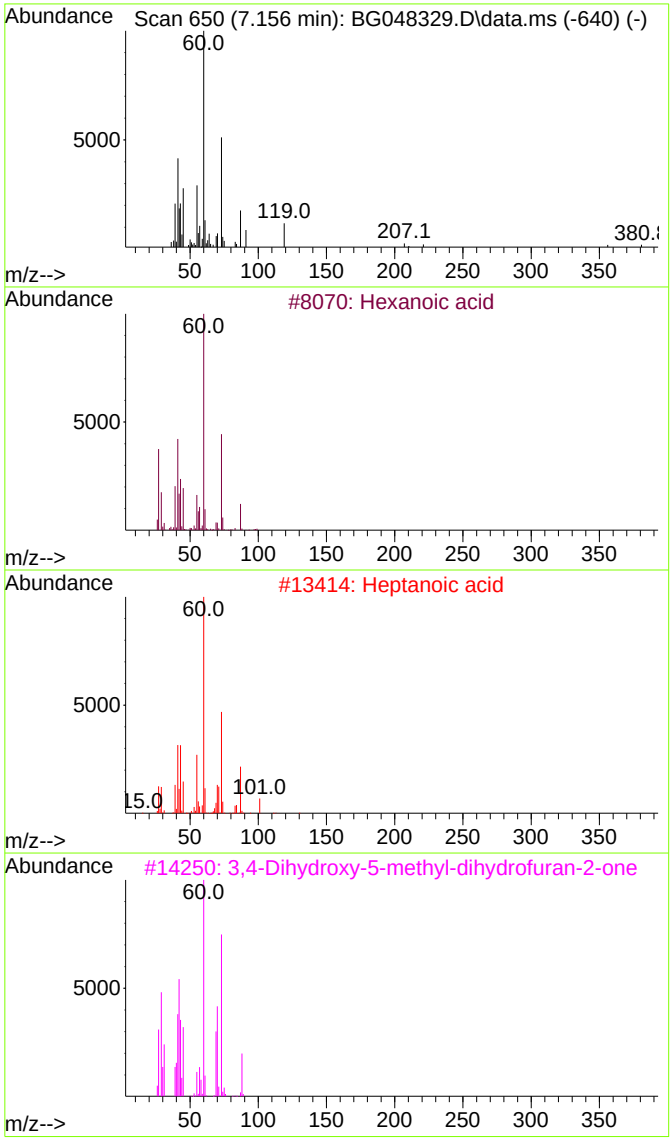
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

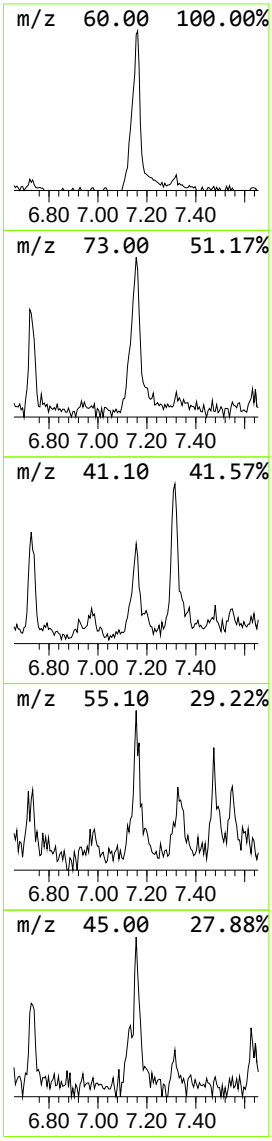
****

Peak Number 4 Hexanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.156	8.20 ng	119481	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	59
2	Heptanoic acid	130	C7H14O2	000111-14-8	59
3	3,4-Dihydroxy-5-methyl-dihydrofu...	132	C5H8O4	1000193-83-1	50
4	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
5	Octanoic acid	144	C8H16O2	000124-07-2	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-41114-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

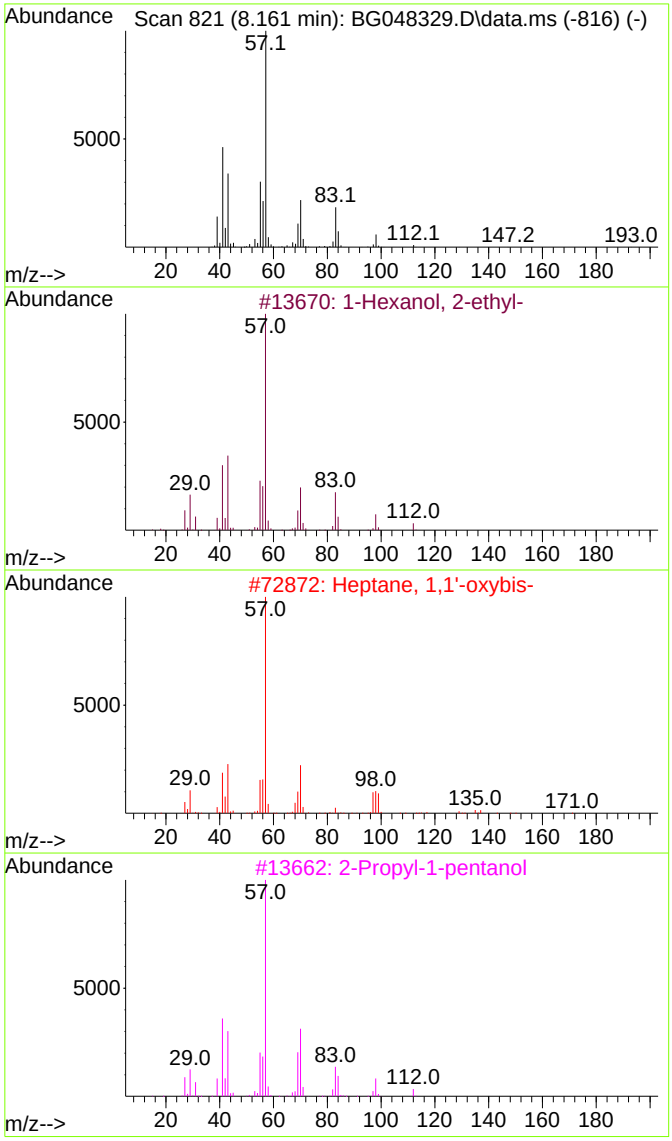
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

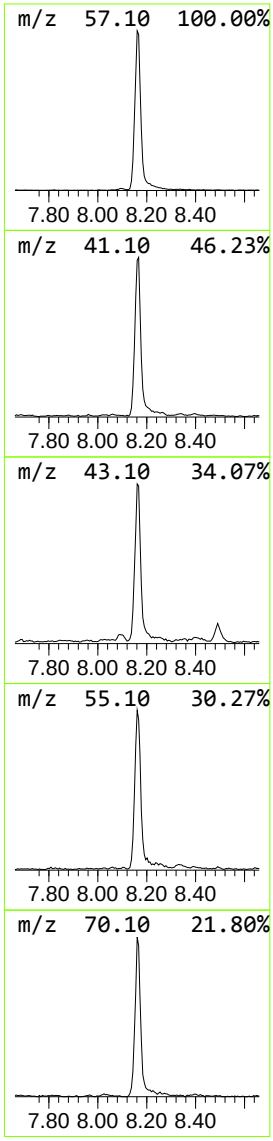
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.161	91.84 ng	1337470	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
4	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	50
5	1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
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Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-41114-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

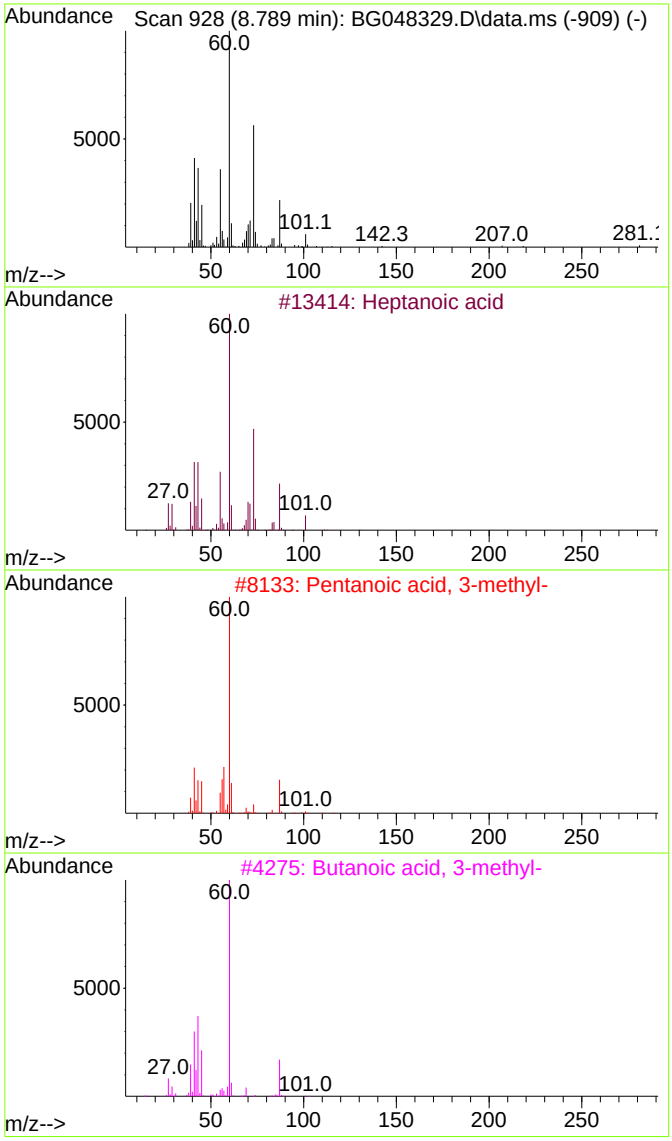
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

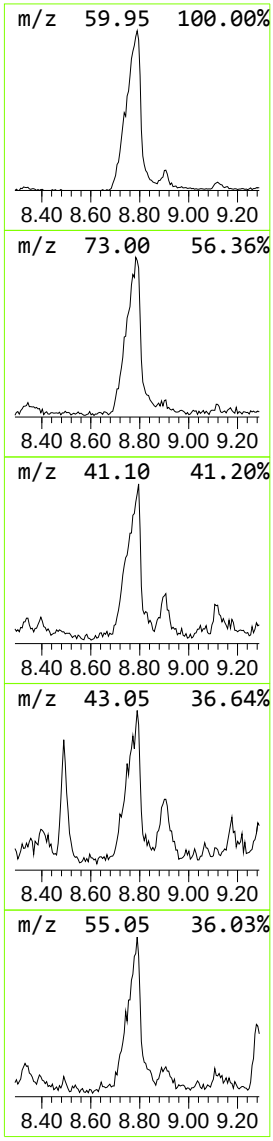
****

Peak Number 6 Heptanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.789	39.71 ng	578331	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	90
2	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	59
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
4	Hexanoic acid	116	C6H12O2	000142-62-1	53
5	Pentanoic acid	102	C5H10O2	000109-52-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
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Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-41114-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

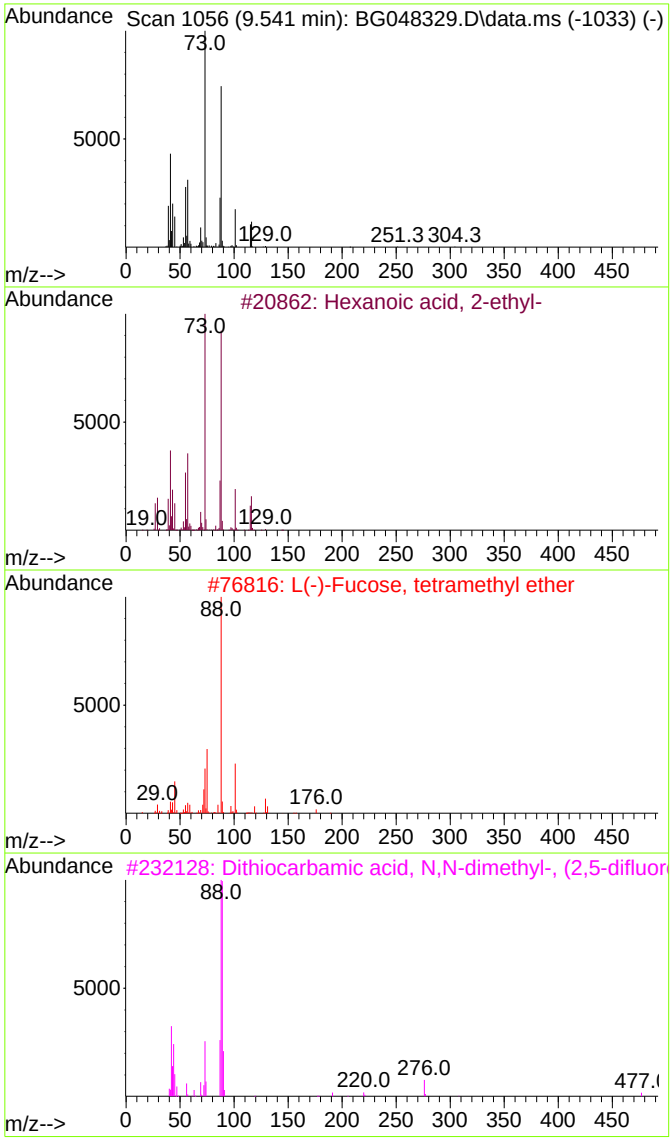
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

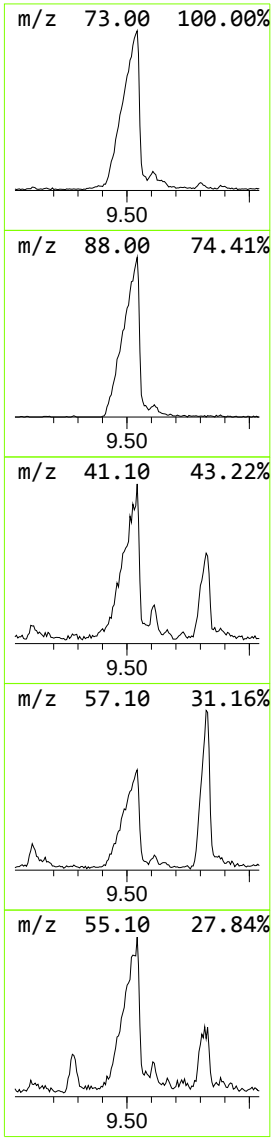
****

Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.541	63.42 ng	1263430	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	L(-)-Fucose, tetramethyl ether	220	C10H20O5	1000332-75-0	40
3	Dithiocarbamic acid, N,N-dimethy...	477	C13H12F9N3S3	1000268-72-7	38
4	Undecanoic acid, 2,6-dimethyl-, ...	228	C14H28O2	055059-28-4	37
5	1,4-Dioxane	88	C4H8O2	000123-91-1	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-41114-15

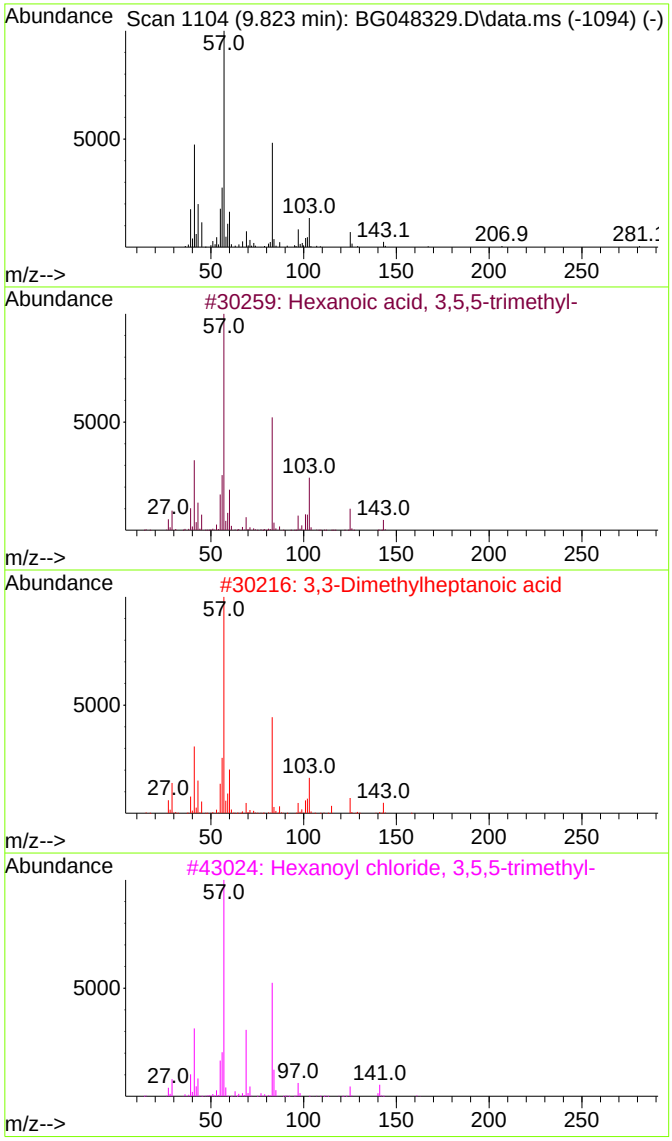
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

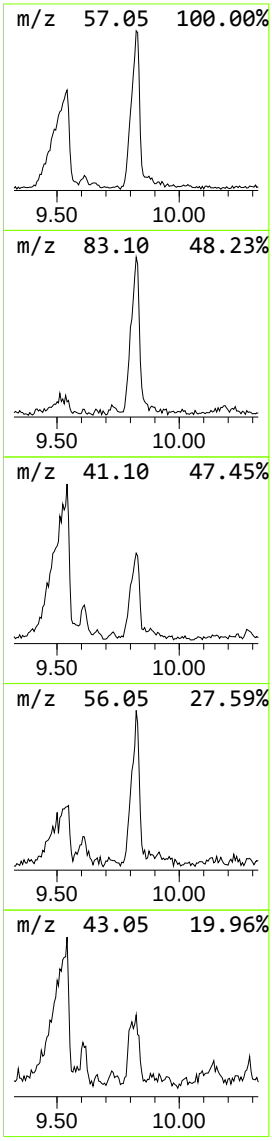
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexanoic acid, 3,5,5-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.823	18.83 ng	375058	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	64
3	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	38
4	4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	38
5	Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	37





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Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-41114-15

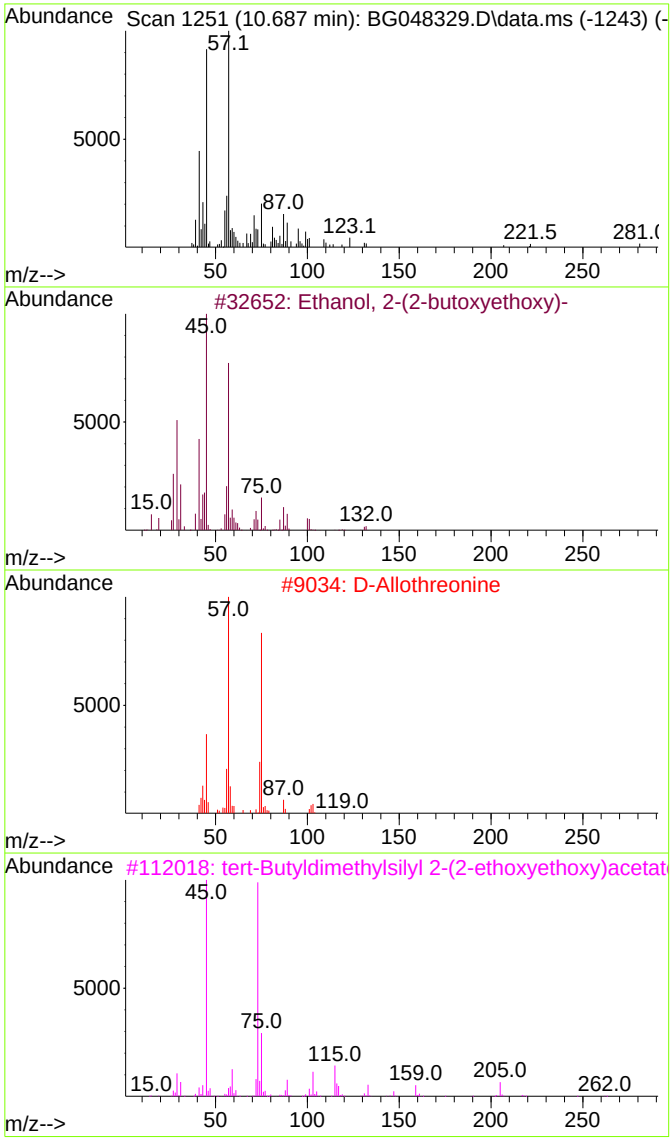
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

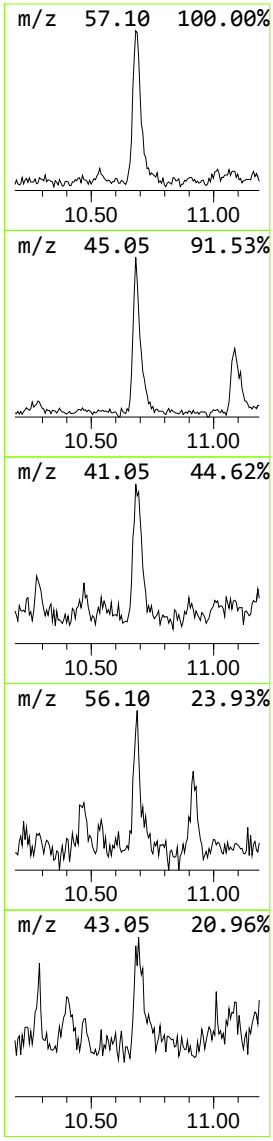
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.687	8.23 ng	163856	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	D-Allothreonine	119	C4H9NO3	024830-94-2	64
3	tert-Butyldimethylsilyl 2-(2-eth...	262	C12H26O4Si	1000366-92-5	50
4	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	50
5	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	50





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Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-41114-15

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

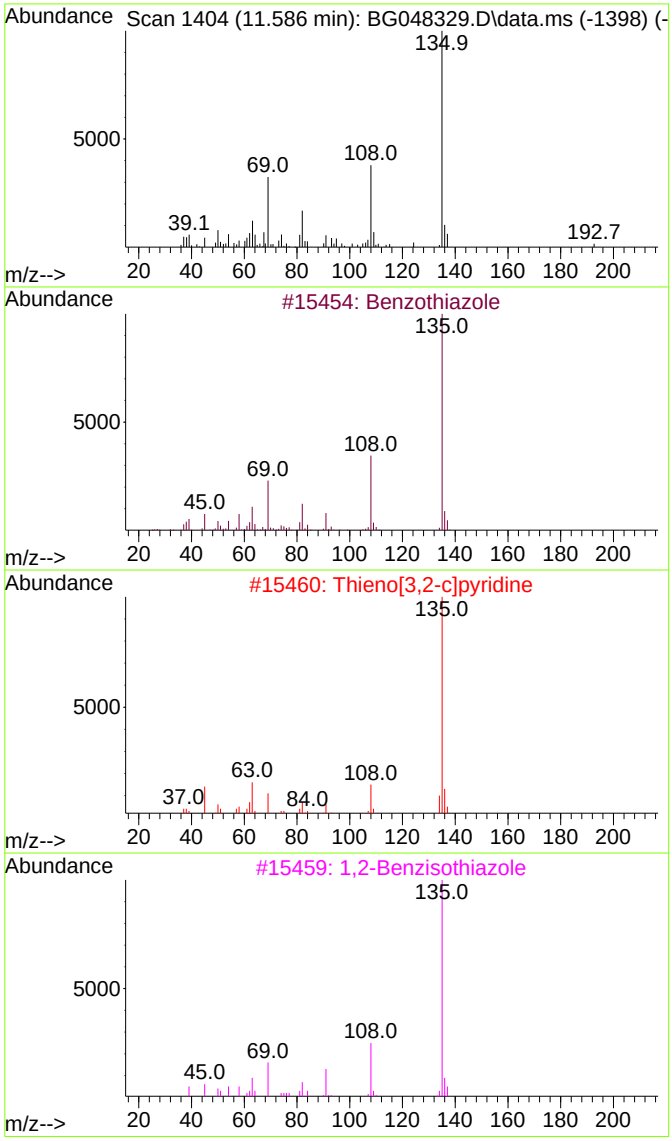
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

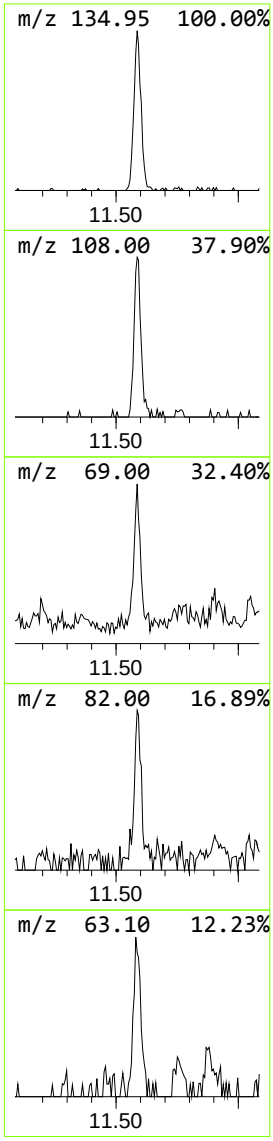
****

Peak Number 10 Benzothiazole Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.586	5.19 ng	103342	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	90
2	Thieno[3,2-c]pyridine	135	C7H5NS	000272-14-0	76
3	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	72
4	Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	000501-00-8	64
5	Adenine	135	C5H5N5	000073-24-5	64





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Instrument : BNA_G
ClientSampleId : COMP-41114-15

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

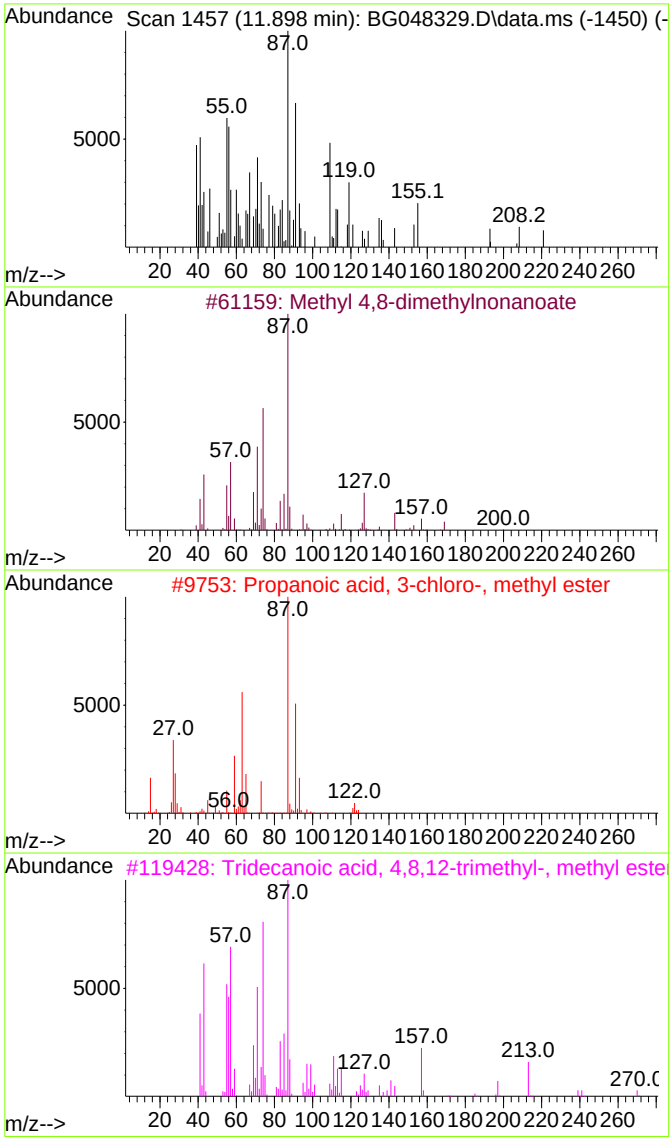
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

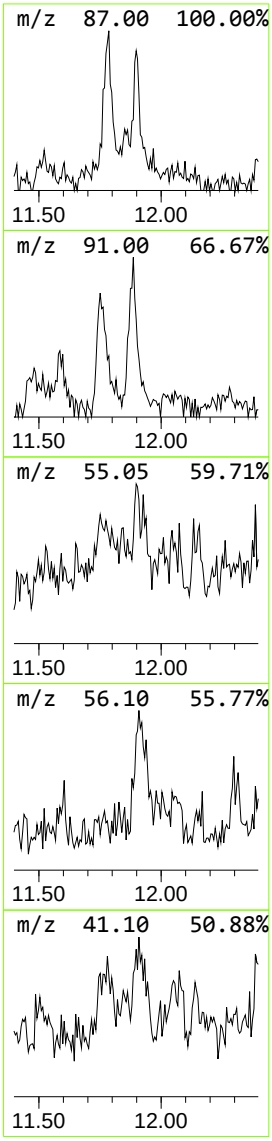
****

Peak Number 11 unknown11.89 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	5.50 ng	109631	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 4,8-dimethylnonanoate	200	C12H24O2	013758-80-0	16
2	Propanoic acid, 3-chloro-, methy...	122	C4H7ClO2	006001-87-2	12
3	Tridecanoic acid, 4,8,12-trimeth...	270	C17H34O2	010339-74-9	12
4	Dimethylphosphinacrylonitryl	113	C5H8NP	077376-93-3	12
5	4-O-Methylmannose	194	C7H14O6	1000130-07-6	12





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Misc :
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Instrument : BNA_G
ClientSampleId : COMP-41114-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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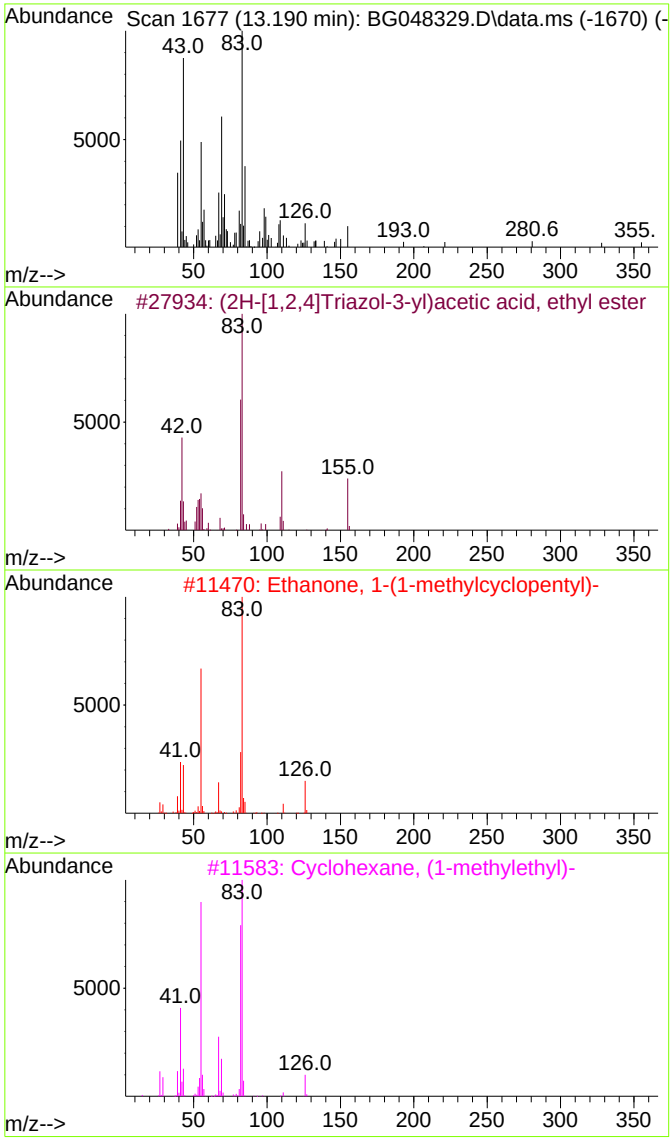
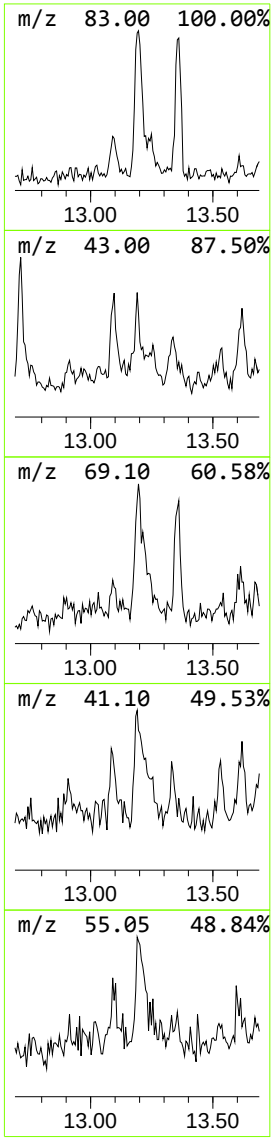
Peak Number 13 unknown13.19 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.190	4.68 ng	136449	Acenaphthene-d10	14.735

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2H-[1,2,4]Triazol-3-yl)acetic a...	155	C6H9N3O2	1000302-73-7	43
2	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	43
3	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	43
4	Cyclohexane, propyl-	126	C9H18	001678-92-8	43
5	Oxalic acid, cyclohexyl decyl ester	312	C18H32O4	1000309-31-2	38





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-41114-15

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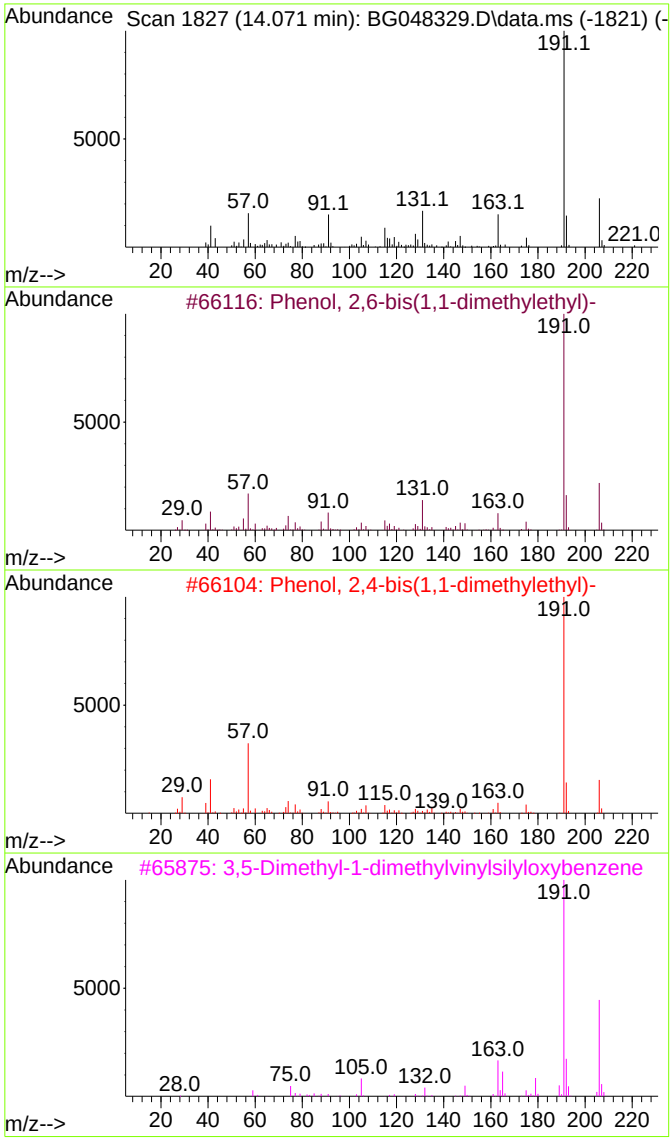
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

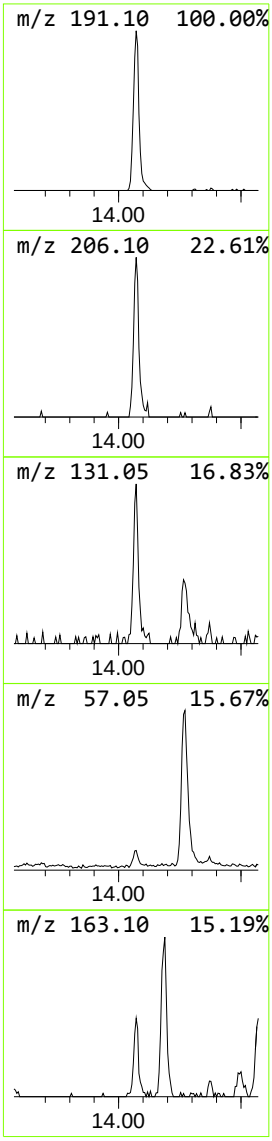
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.071	5.74 ng	167213	Acenaphthene-d10	14.735

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	91
2	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	87
3	3,5-Dimethyl-1-dimethylvinylsily...	206	C12H18OSi	1000307-91-8	72
4	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	72
5	Benzeneacetic acid, 4-(1,1-dimet...	206	C13H18O2	003549-23-3	72





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Instrument : BNA_G
ClientSampleId : COMP-41114-15

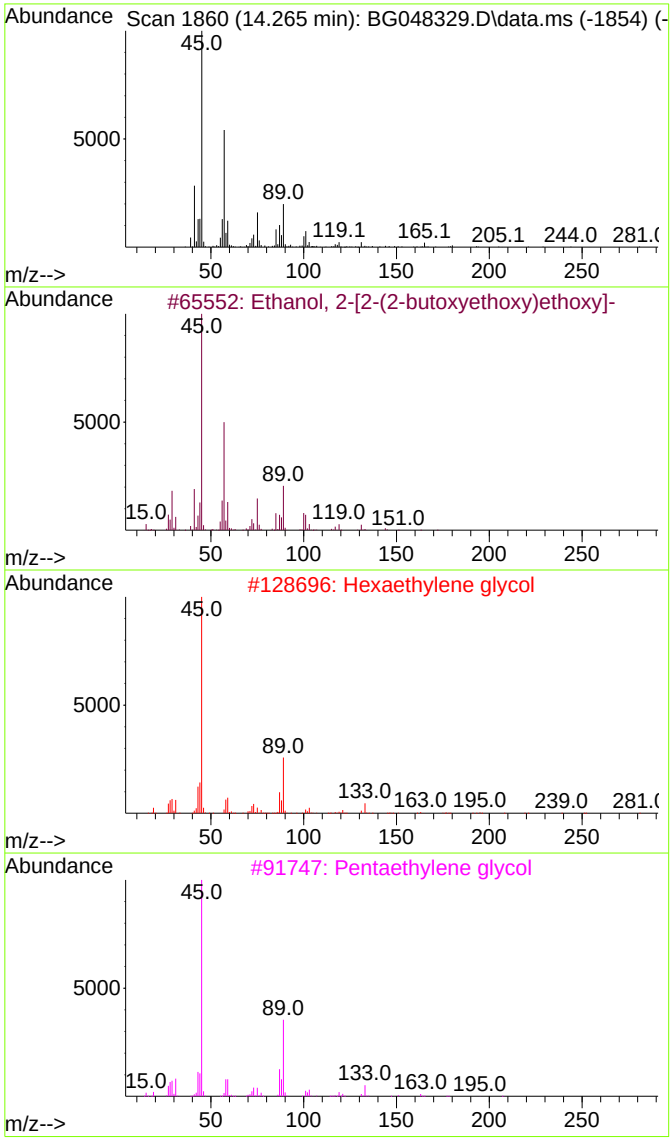
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

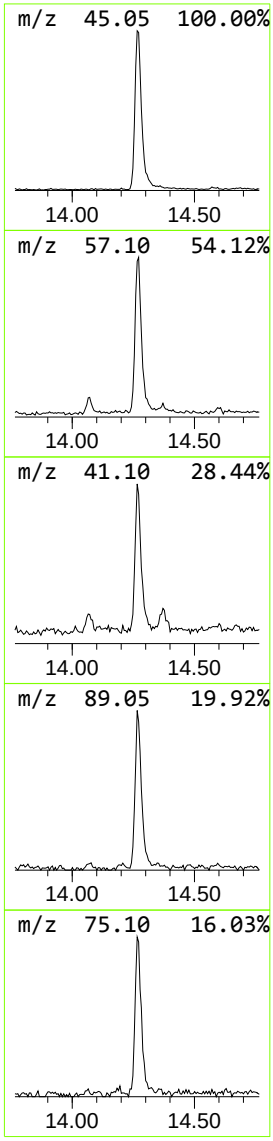
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.265	19.47 ng	567353	Acenaphthene-d10	14.735

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	90
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	80
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	80
4	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	78
5	Triethylene glycol	150	C6H14O4	000112-27-6	72





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Operator : CG/JU
Sample : M1507-06
Misc :
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Instrument :
BNA_G
ClientSampleId :
COMP-41114-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

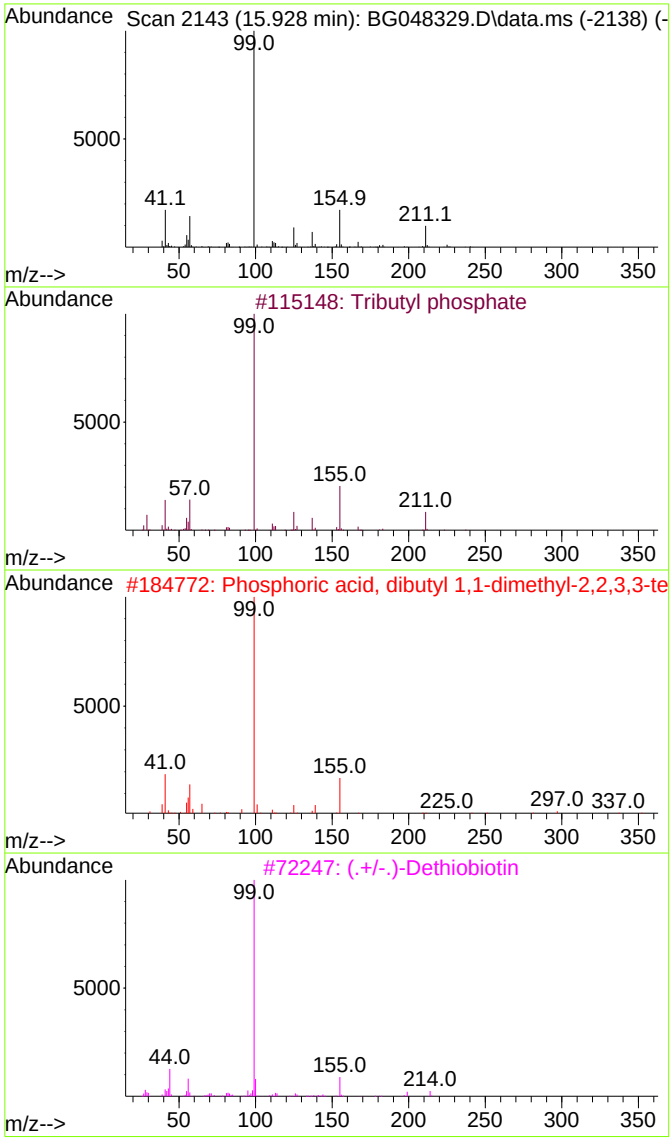
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

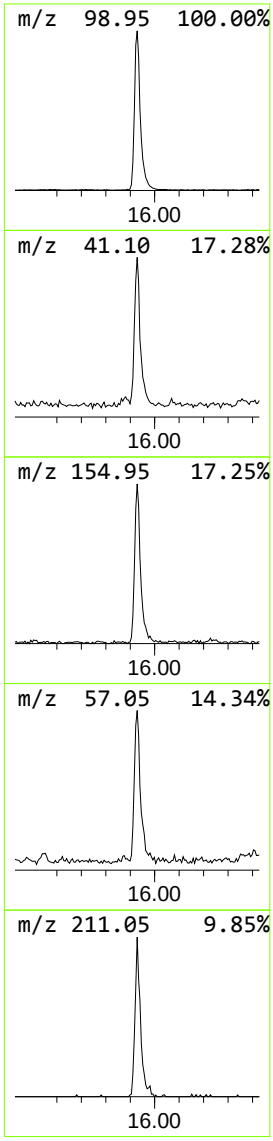
****

Peak Number 16 Tributyl phosphate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.928	21.76 ng	634081	Acenaphthene-d10	14.735

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	91
2	Phosphoric acid, dibutyl 1,1-dim...	352	C13H25F4O4P	1000298-93-9	56
3	(.+/-.)-Dethiobiotin	214	C10H18N2O3	000636-20-4	40
4	Phosphoric acid, dibutyl 3-trifl...	348	C14H28F3O4P	1000298-93-8	40
5	tri-n-Amylphosphate	308	C15H33O4P	002528-38-3	33





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Misc :
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Instrument : BNA_G
ClientSampleId : COMP-41114-15

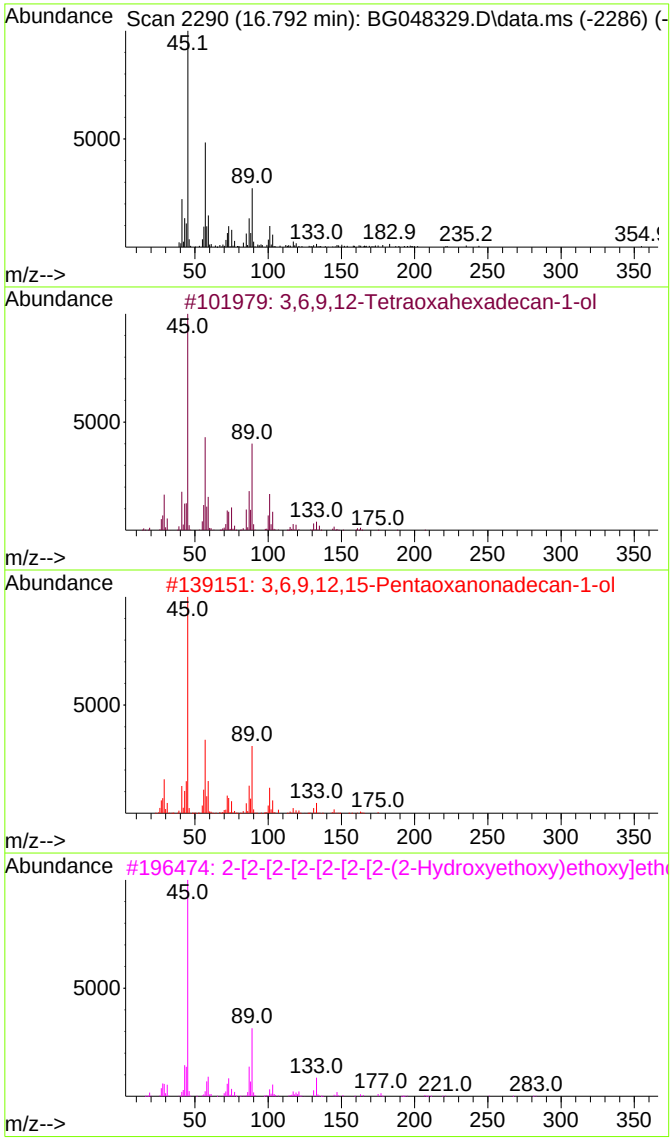
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

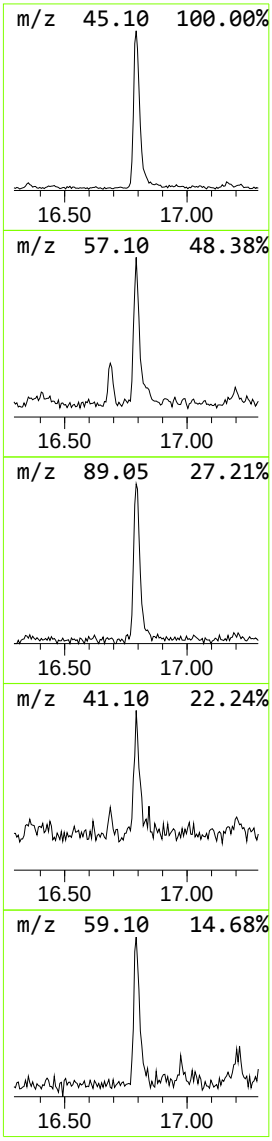
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 3,6,9,12-Tetraoxahexadecan-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.792	7.44 ng	241713	Phenanthrene-d10	17.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	91
2	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	91
3	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	86
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	86
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	78





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Instrument : BNA_G
ClientSampleId : COMP-41114-15

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

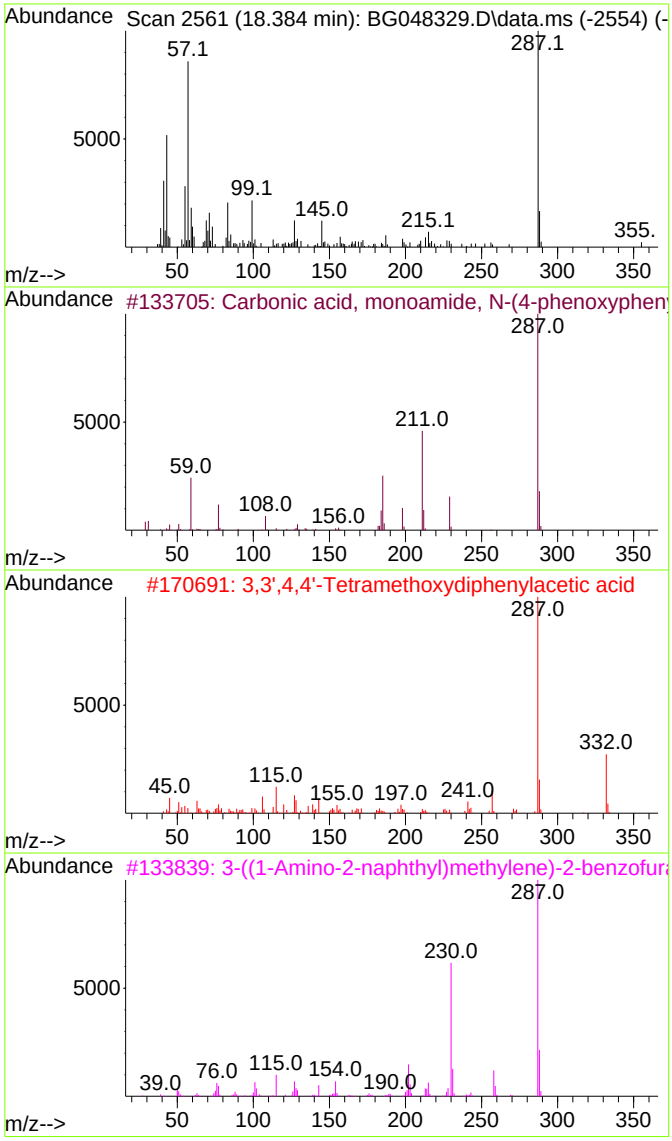
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

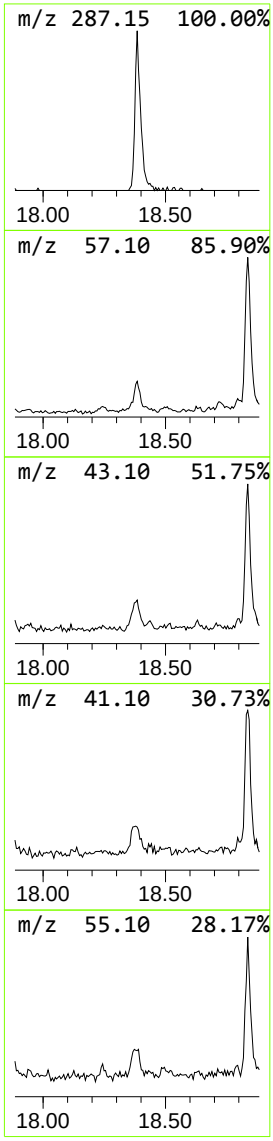
****

Peak Number 18 unknown18.38 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.384	4.96 ng	161228	Phenanthrene-d10	17.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, monoamide, N-(4-p...	287	C16H17NO4	1000340-02-1	46
2	3,3',4,4'-Tetramethoxydiphenylac...	332	C18H20O6	020153-24-6	43
3	3-((1-Amino-2-naphthyl)methylene...	287	C19H13NO2	1000332-19-1	43
4	3-((1-Amino-2-naphthyl)methylene...	287	C19H13NO2	1000332-19-2	43
5	p-Methoxybenzylidene p-biphenyla...	287	C20H17NO	025543-63-9	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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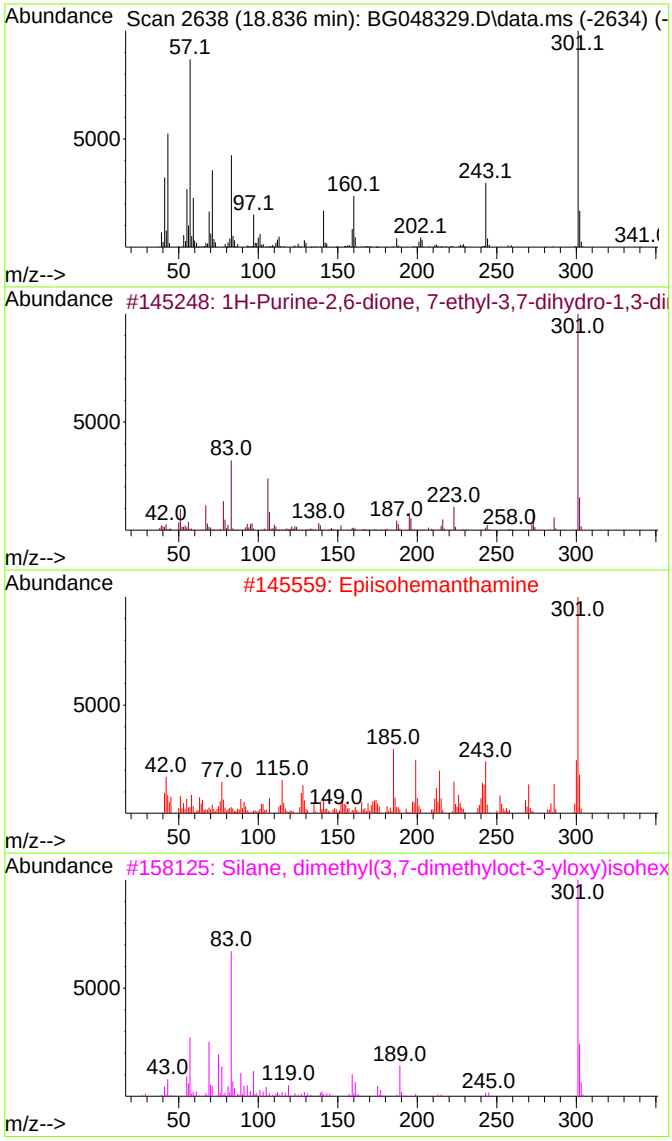
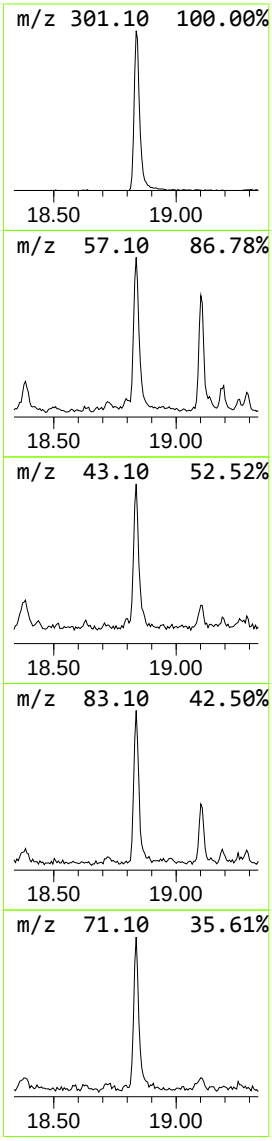
Peak Number 19 unknown18.83 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.836	23.84 ng	774692	Phenanthrene-d10	17.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Purine-2,6-dione, 7-ethyl-3,7...	301	C14H15N5O3	1000337-95-2	43
2	Epiisohemanthamine	301	C17H19NO4	006883-68-7	35
3	Silane, dimethyl(3,7-dimethyloct...	316	C18H40O2Si	1000346-78-2	27
4	Pyrrole, 4-acetyl-5-methyl-2-phe...	301	C21H19NO	1000150-87-2	25
5	Silane, diethyl(3-methylpentylox...	330	C19H42O2Si	1000363-48-9	25





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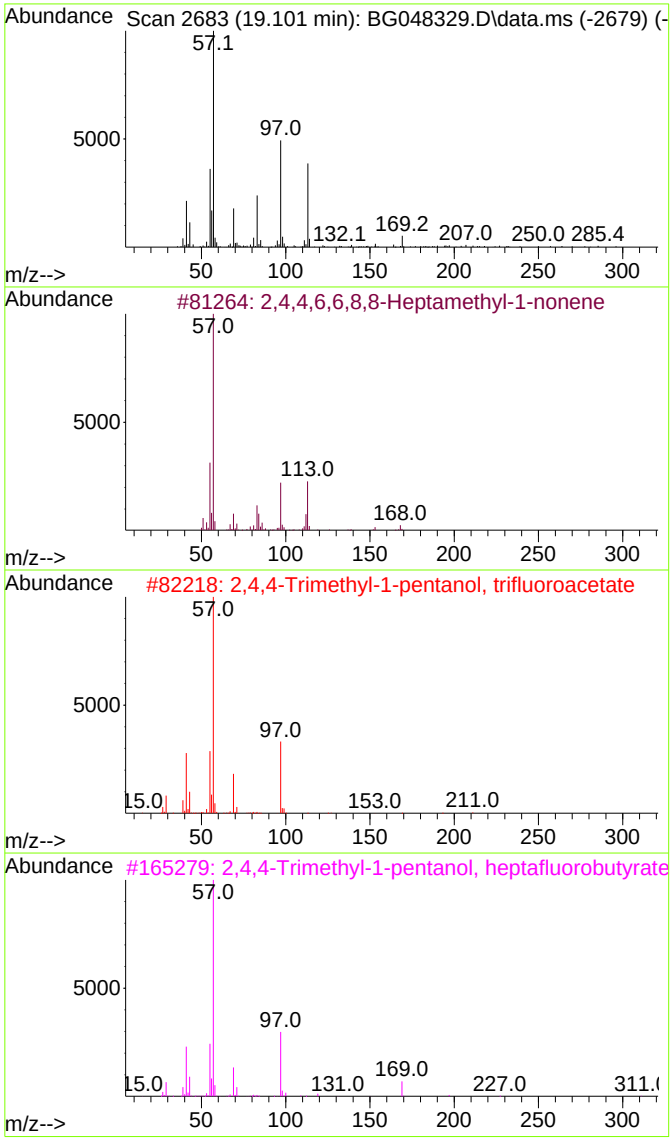
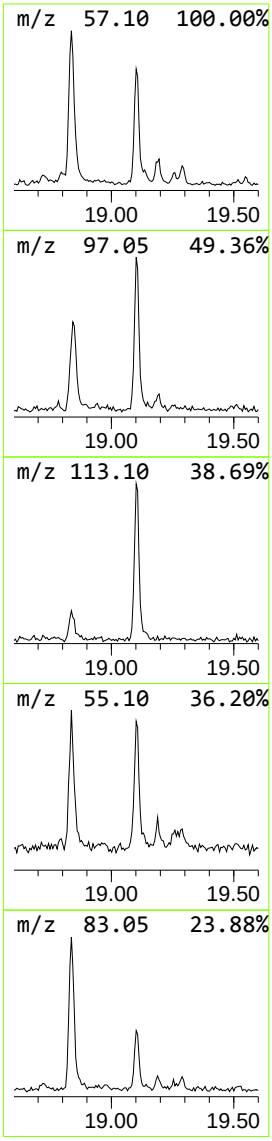
Peak Number 20 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.101	6.90 ng	224147	Phenanthrene-d10	17.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	56
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	32
3	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	32
4	4-Methylnonanoic acid	172	C10H20O2	045019-28-1	28
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048329.D
Acq On : 4 Mar 2021 15:23
Operator : CG/JU
Sample : M1507-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-41114-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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
Ethanol, 2-butoxy-	6.175	142.2	ng	2070380	1	8.102	291247	20.0
(R)-(-)-2,2-Dim...	6.727	15.4	ng	223478	1	8.102	291247	20.0
Hexanoic acid	7.156	8.2	ng	119481	1	8.102	291247	20.0
1-Hexanol, 2-et...	8.161	91.8	ng	1337470	1	8.102	291247	20.0
Heptanoic acid	8.789	39.7	ng	578331	1	8.102	291247	20.0
Hexanoic acid, ...	9.541	63.4	ng	1263430	2	10.922	398420	20.0
Hexanoic acid, ...	9.823	18.8	ng	375058	2	10.922	398420	20.0
Ethanol, 2-(2-b...	10.687	8.2	ng	163856	2	10.922	398420	20.0
Benzothiazole	11.586	5.2	ng	103342	2	10.922	398420	20.0
unknown11.89	11.898	5.5	ng	109631	2	10.922	398420	20.0
unknown13.19	13.190	4.7	ng	136449	3	14.735	582755	20.0
Phenol, 2,6-bis...	14.071	5.7	ng	167213	3	14.735	582755	20.0
Ethanol, 2-[2-(...	14.265	19.5	ng	567353	3	14.735	582755	20.0
Tributyl phosphate	15.928	21.8	ng	634081	3	14.735	582755	20.0
3,6,9,12-Tetrao...	16.792	7.4	ng	241713	4	17.485	649891	20.0
unknown18.38	18.384	5.0	ng	161228	4	17.485	649891	20.0
unknown18.83	18.836	23.8	ng	774692	4	17.485	649891	20.0
2,4,4,6,6,8,8-H...	19.101	6.9	ng	224147	4	17.485	649891	20.0