LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050825\
Data File : BM050149.D
Acq On : 08 May 2025 16:39
Operator : RC/JU
Sample : Q1968-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MH-N

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_M\Methods\8270-BM042825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM050149.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.481	81	84	97	rBV	100681	171436	1.82%	0.340%
2	4.863	313	319	330	rBV	265069	390776	4.15%	0.775%
3	5.334	393	399	415	rBV	2696712	4214259	44.73%	8.357%
4	6.934	664	671	698	rBV	2126205	4215989	44.75%	8.360%
5	7.740	801	808	818	rBV	870077	1415396	15.02%	2.807%
6	8.904	998	1006	1023	rBV	1313988	2638336	28.00%	5.232%
7	10.539	1276	1284	1306	rBV	866648	1778668	18.88%	3.527%
8	11.310	1407	1415	1432	rBV2	72661	266301	2.83%	0.528%
9	13.004	1695	1703	1725	rBV	3886226	6469190	68.67%	12.829%
10	14.392	1931	1939	1958	rBV	1434216	2414997	25.63%	4.789%
11	14.616	1967	1977	1985	rBV	86609	213300	2.26%	0.423%
12	15.763	2166	2172	2184	rBV	74971	147068	1.56%	0.292%
13	15.892	2187	2194	2214	rBV	2981450	5167602	54.85%	10.248%
14	17.145	2400	2407	2423	rBV2	1578000	2685796	28.51%	5.326%
15	18.039	2553	2559	2575	rBV	517052	1093774	11.61%	2.169%
16	19.221	2745	2760	2762	rBV7	179714	644512	6.84%	1.278%
17	19.315	2773	2776	2795	rVB3	290202	632158	6.71%	1.254%
18	19.762	2847	2852	2863	rBV	7509024	9421087	100.00%	18.682%
19	20.462	2968	2971	2979	rBV	95636	121624	1.29%	0.241%
20	21.051	3068	3071	3079	rBV	222374	312502	3.32%	0.620%
21	21.386	3122	3128	3139	rBV	1908840	2963683	31.46%	5.877%
22	24.374	3629	3636	3654	rVB	1102498	3049377	32.37%	6.047%

Sum of corrected areas: 50427831

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM050825\
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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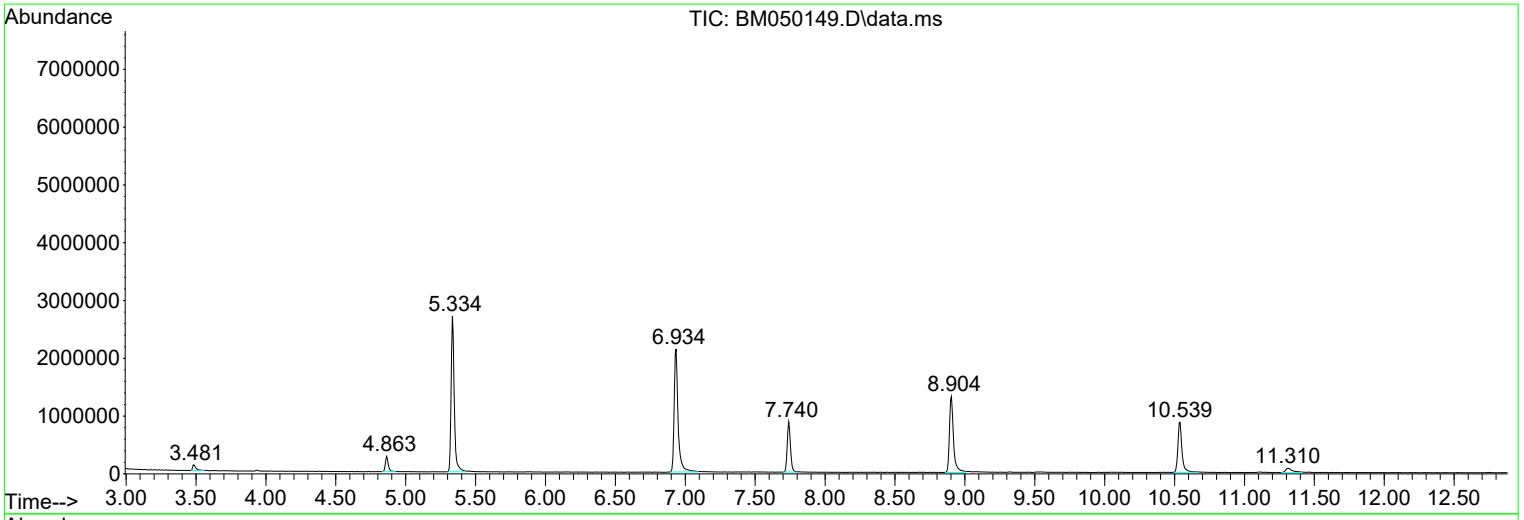
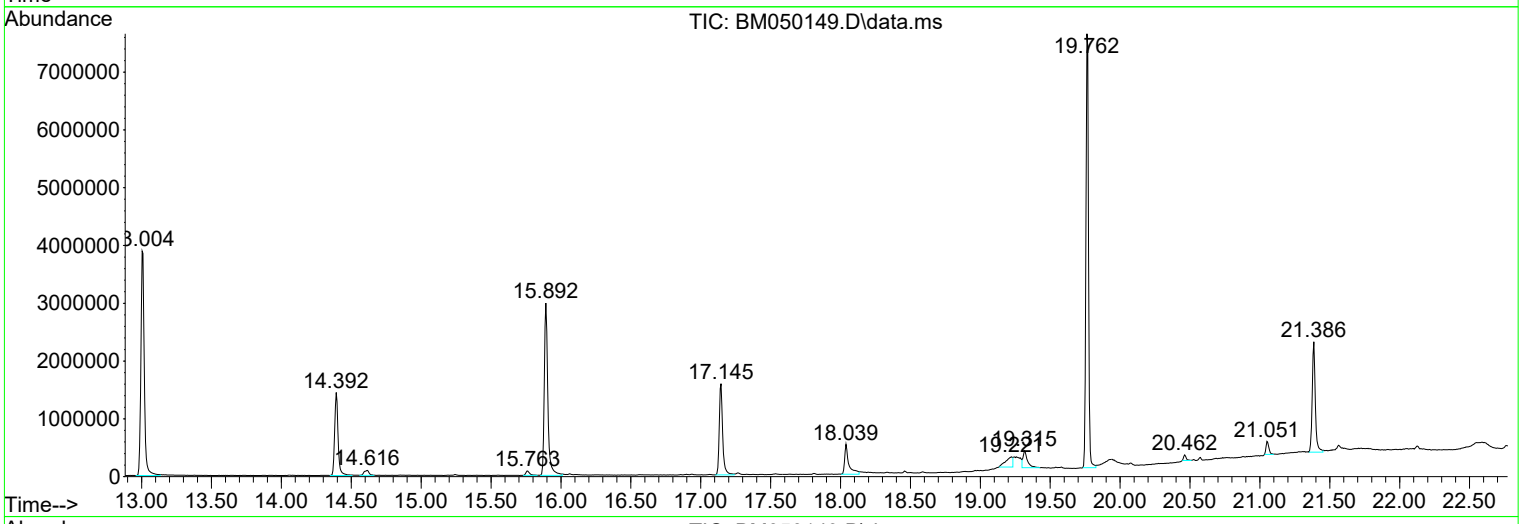
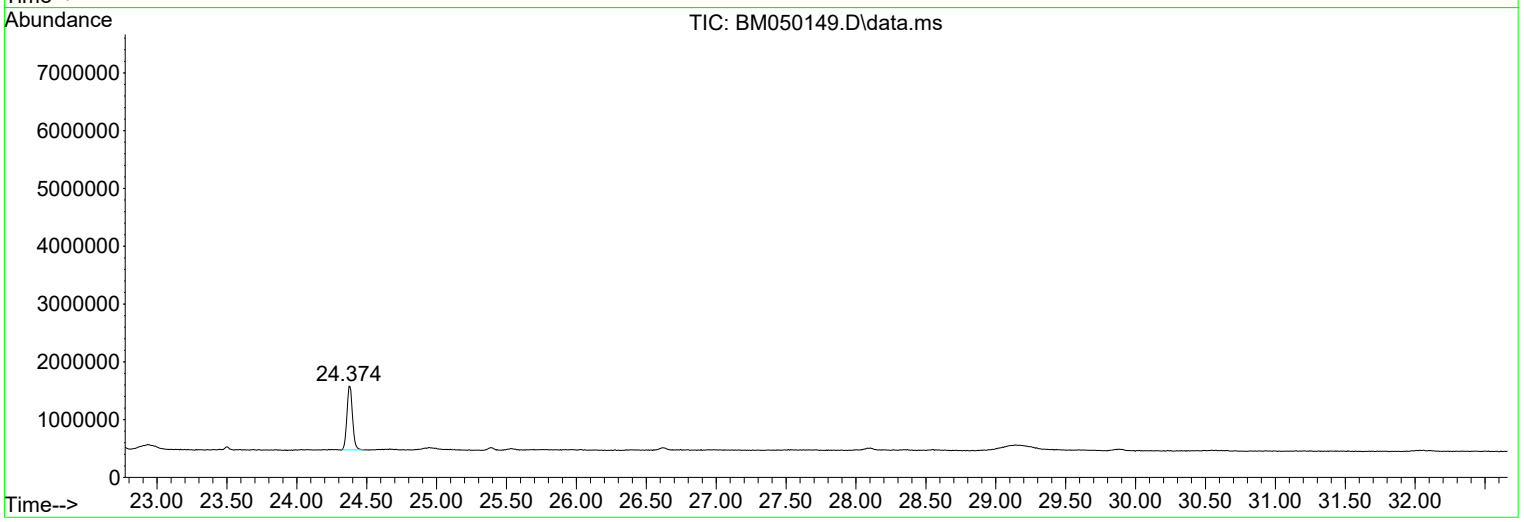
ClientSampleId :
MH-N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.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 : BM050149.D
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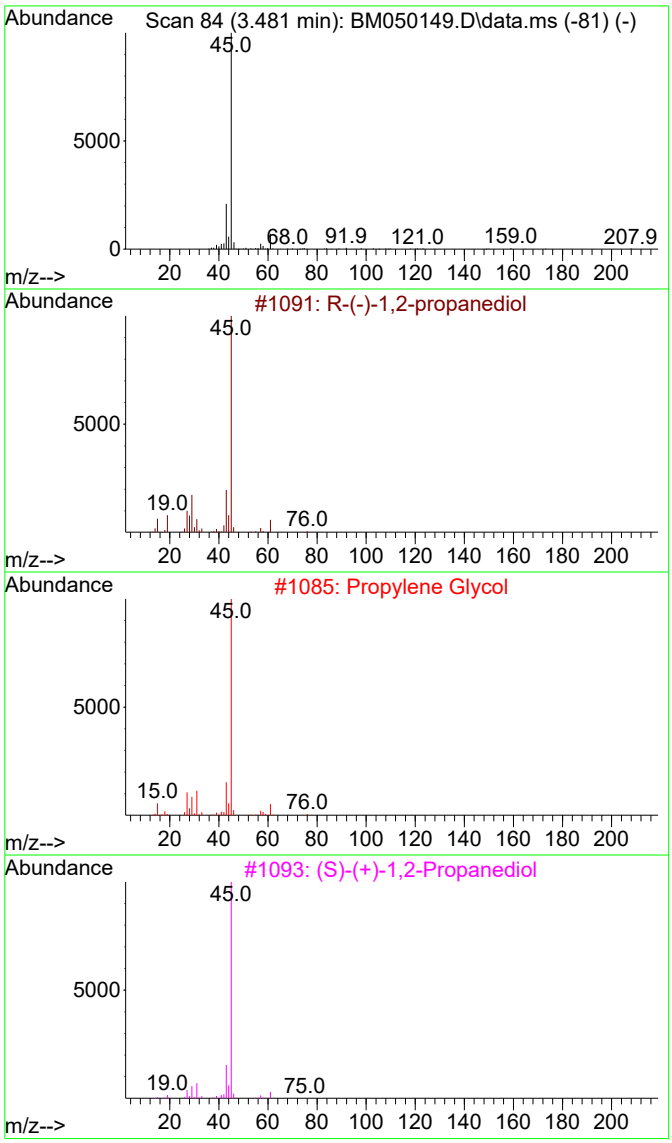
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

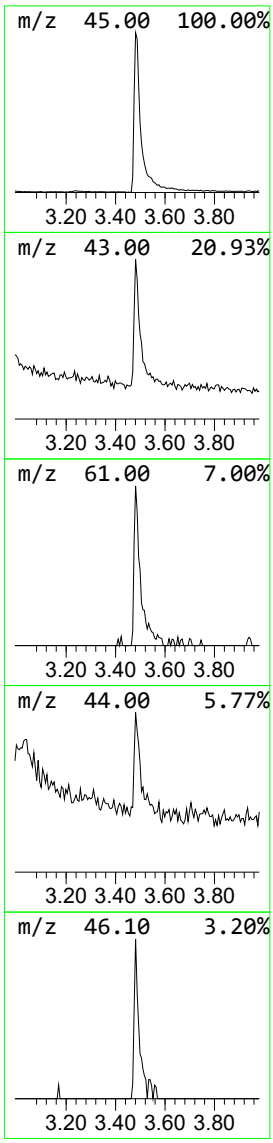
****

Peak Number 1 unknown3.481 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.481	2.42 ng	171436	1,4-Dichlorobenzene-d4	7.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
2	Propylene Glycol	76	C3H8O2	000057-55-6	40
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	39
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	2-Butanol	74	C4H10O	000078-92-2	9





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Sample : Q1968-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MH-N

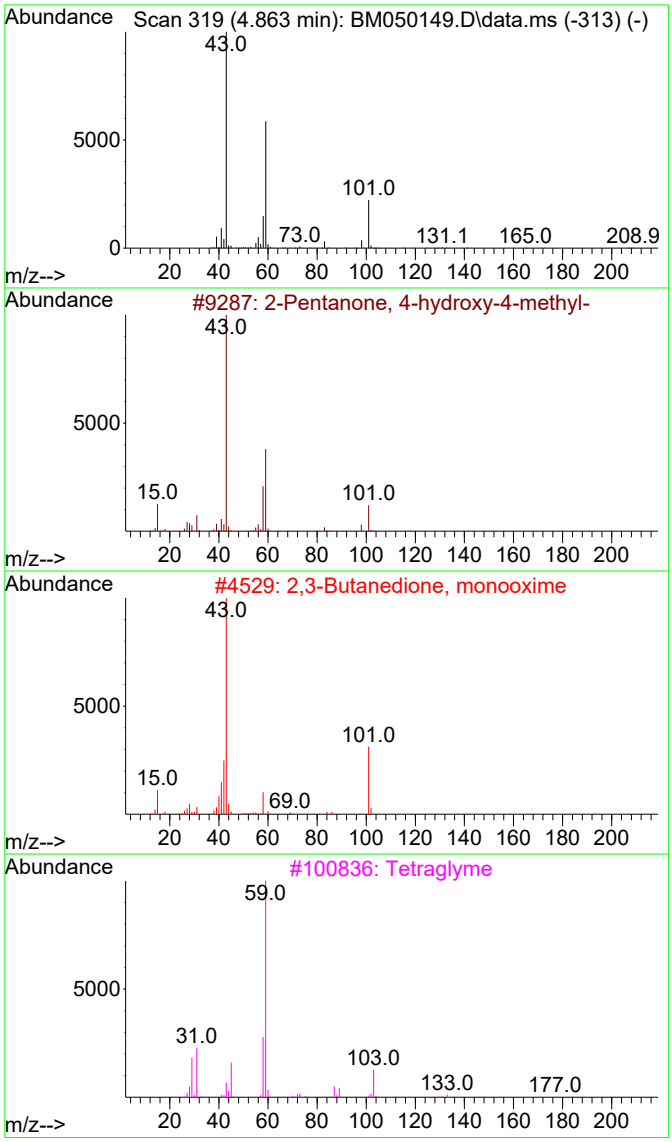
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

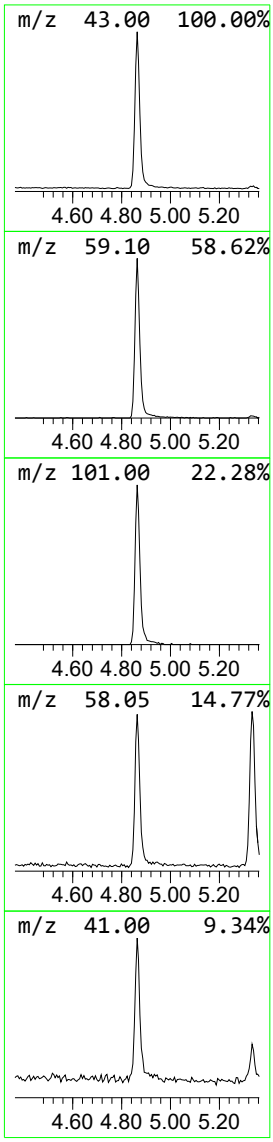
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.863	5.52 ng	390776	1,4-Dichlorobenzene-d4	7.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Tetraglyme	222	C10H22O5	000143-24-8	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Hexanamide	115	C6H13NO	000628-02-4	9





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Operator : RC/JU
Sample : Q1968-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MH-N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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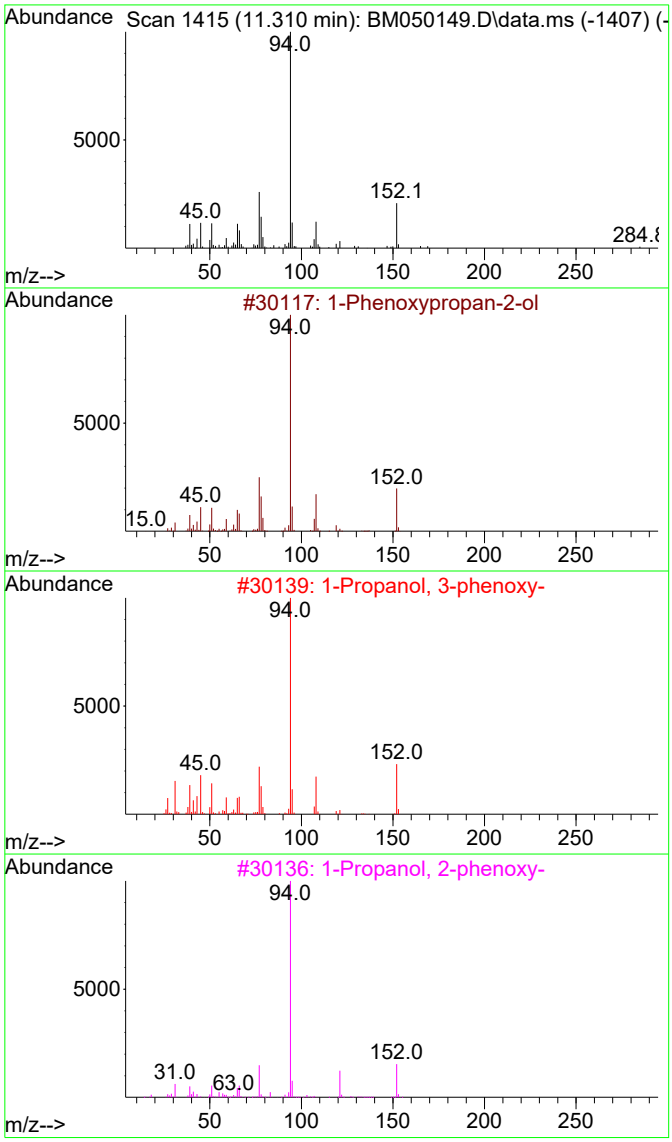
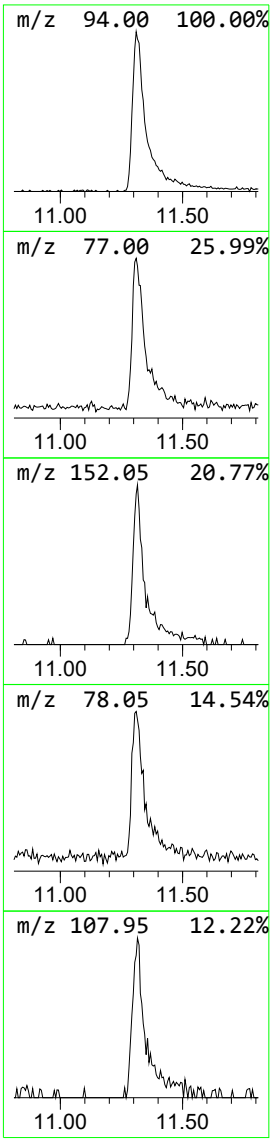
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.310	2.99 ng	266301	Naphthalene-d8	10.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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Sample : Q1968-01
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MH-N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

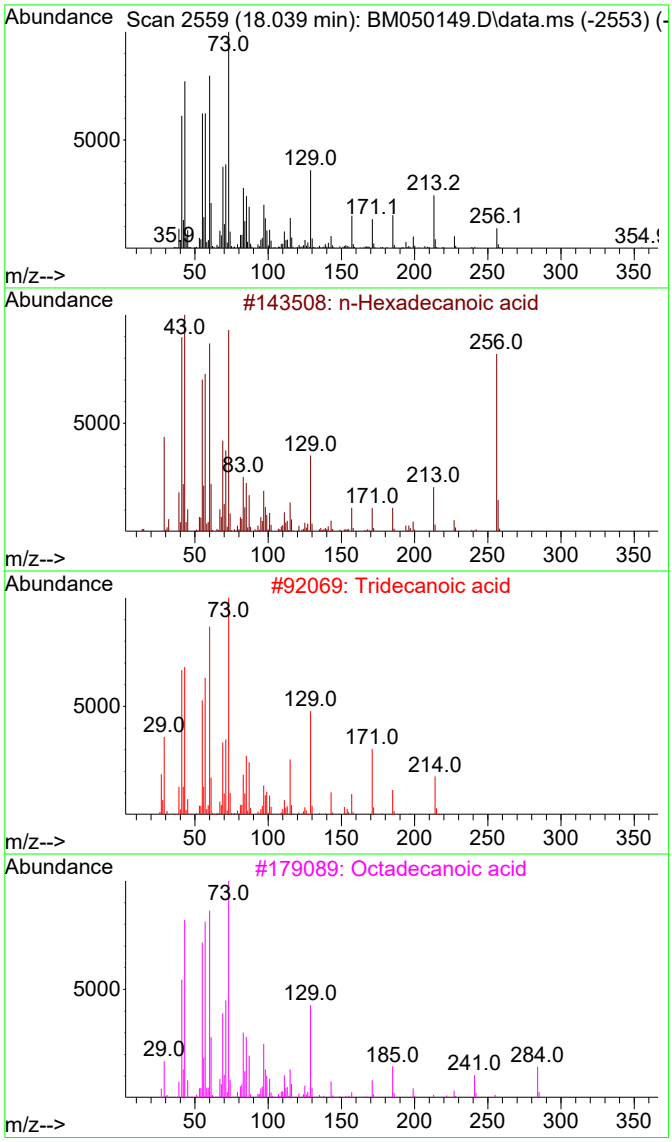
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

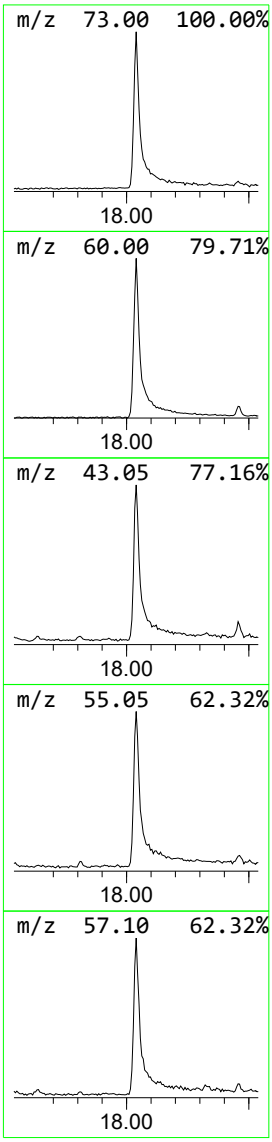
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.039	8.14 ng	1093770	Phenanthrene-d10	17.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	81





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Operator : RC/JU
Sample : Q1968-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MH-N

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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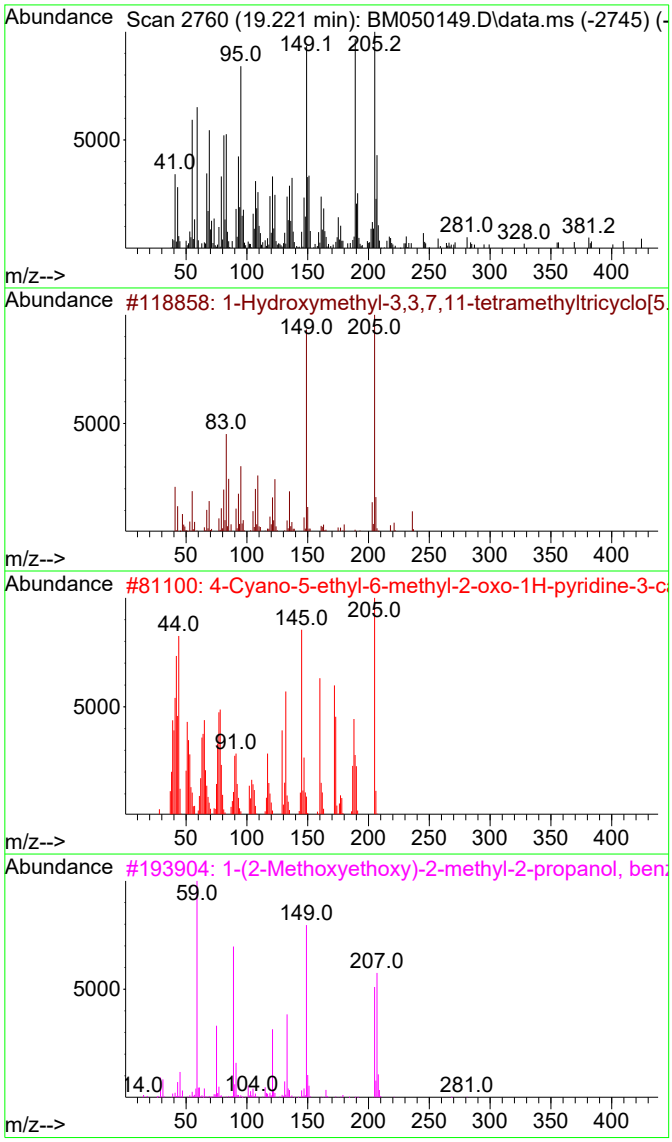
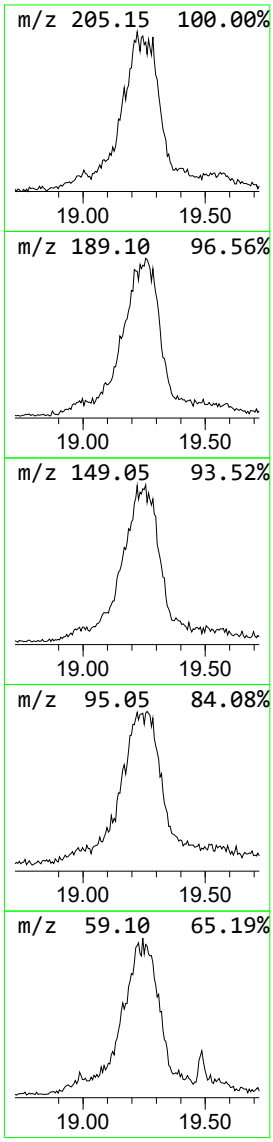
Peak Number 5 unknown19.221 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.221	4.80 ng	644512	Phenanthrene-d10	17.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hydroxymethyl-3,3,7,11-tetrame...	236	C16H28O	1000140-33-0	27
2	4-Cyano-5-ethyl-6-methyl-2-oxo-1...	205	C10H11N3O2	1000435-90-0	25
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	296	C16H28O3Si	1000376-05-8	22
4	7-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-91-0	14
5	3-Hydroxy-2,3-dihydro-1H-indol-2...	233	C12H11NO4	1000502-99-4	11





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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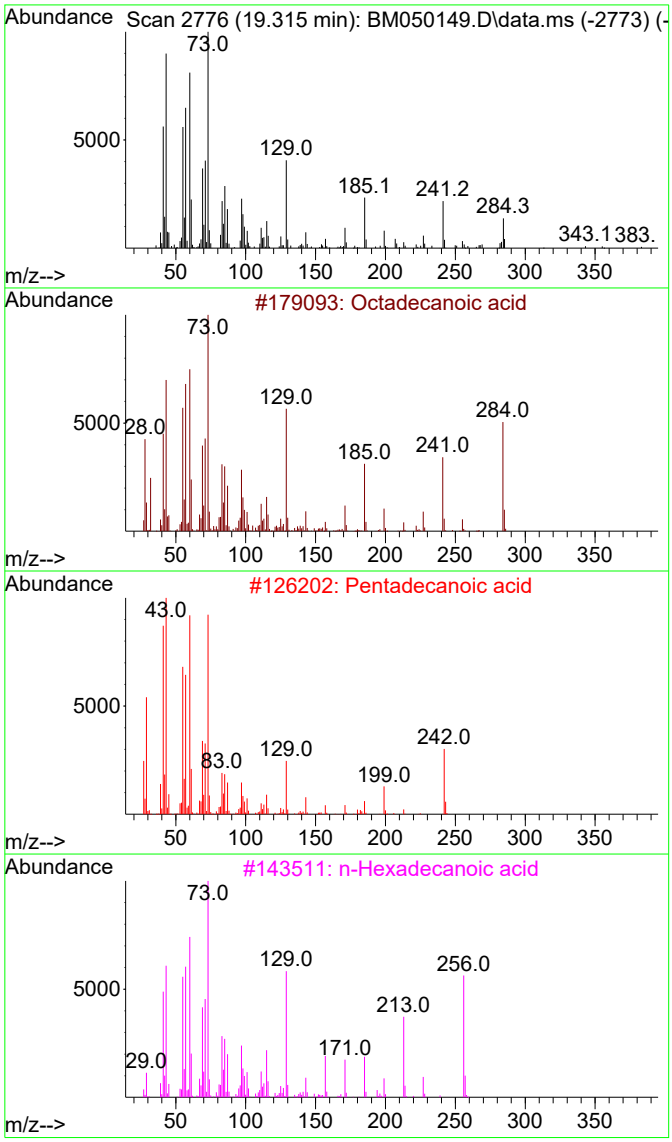
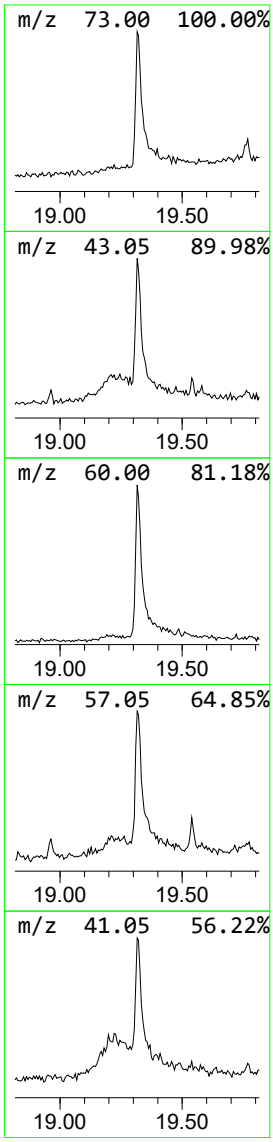
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.315	4.27 ng	632158	Chrysene-d12	21.386

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	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	78





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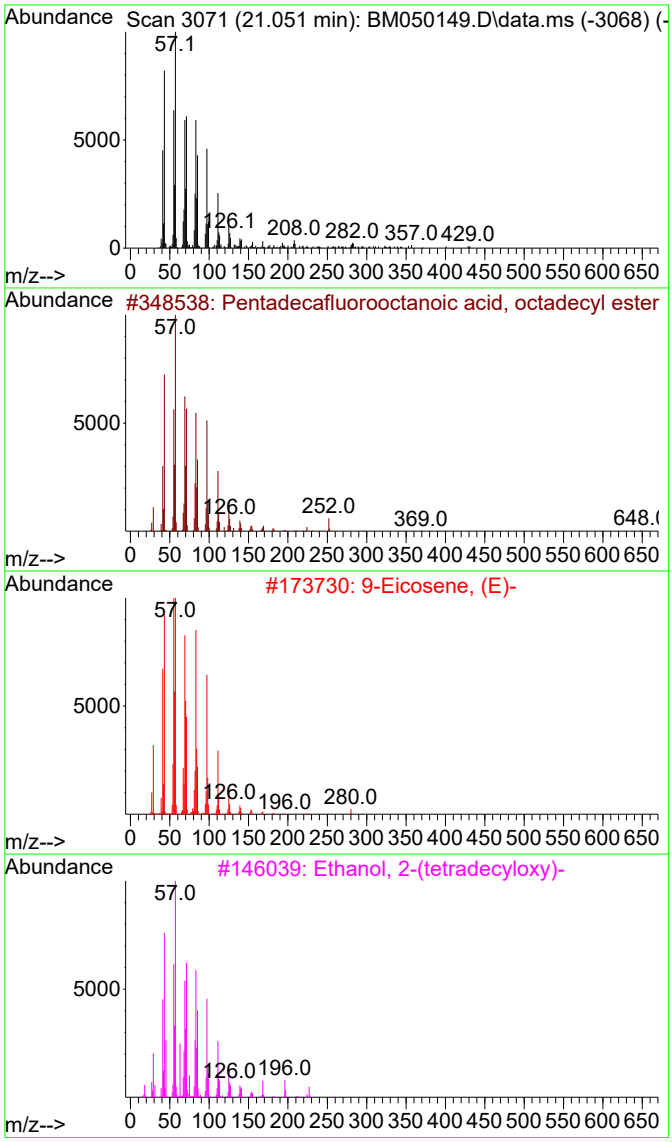
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

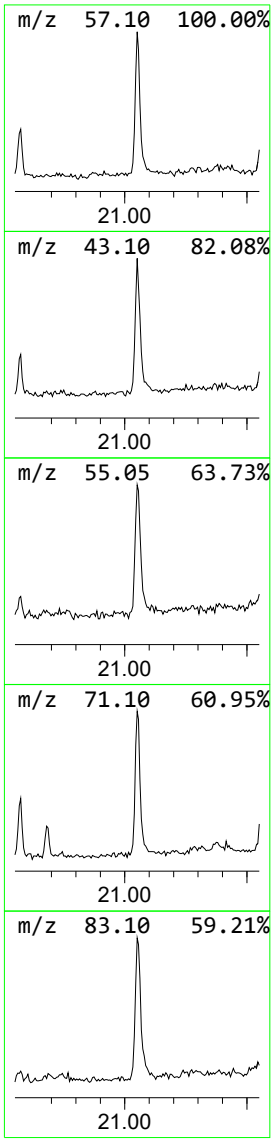
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	2.11 ng	312502	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	92
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	76
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	76





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
unknown3.481	3.481	2.4	ng	171436	1	7.740	1415400	20.0
2-Pentanone, 4-...	4.863	5.5	ng	390776	1	7.740	1415400	20.0
1-Phenoxypropan...	11.310	3.0	ng	266301	2	10.534	1778670	20.0
n-Hexadecanoic ...	18.039	8.1	ng	1093770	4	17.145	2685800	20.0
unknown19.221	19.221	4.8	ng	644512	4	17.145	2685800	20.0
Octadecanoic acid	19.315	4.3	ng	632158	5	21.386	2963680	20.0
Pentadecafluoro...	21.051	2.1	ng	312502	5	21.386	2963680	20.0