LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139036.D
Acq On : 15 Aug 2024 22:16
Operator : RC/JU
Sample : P3573-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-856-J-S0-3-3.5-080924

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_F\Methods\8270-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139036.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	14	rVB	572482	683932	63.85%	9.027%
2	3.398	217	222	233	rBV	10033	32003	2.99%	0.422%
3	5.063	500	505	517	rVB	39946	62810	5.86%	0.829%
4	5.469	569	574	595	rBV	697487	968102	90.39%	12.778%
5	6.481	741	746	773	rBV	755081	1019985	95.23%	13.463%
6	6.833	802	806	814	rVB	196384	237705	22.19%	3.137%
7	7.398	897	902	915	rBV	481753	646103	60.32%	8.528%
8	7.663	943	947	954	rBB	8301	13873	1.30%	0.183%
9	8.116	1019	1024	1035	rBV	253979	314473	29.36%	4.151%
10	8.433	1074	1078	1085	rBV	32639	49268	4.60%	0.650%
11	9.186	1201	1206	1211	rBV	882429	1071081	100.00%	14.137%
12	9.869	1317	1322	1332	rVB	268341	343095	32.03%	4.529%
13	9.957	1332	1337	1343	rBV	23061	33532	3.13%	0.443%
14	10.657	1451	1456	1470	rBV	471167	609122	56.87%	8.040%
15	11.351	1569	1574	1584	rBV	242813	318467	29.73%	4.203%
16	12.933	1838	1843	1848	rBV	606690	739927	69.08%	9.766%
17	13.827	1989	1995	2014	rBV3	13787	44775	4.18%	0.591%
18	13.998	2019	2024	2032	rVV	136616	179566	16.76%	2.370%
19	14.939	2180	2184	2189	rVB	23159	31602	2.95%	0.417%
20	15.462	2267	2273	2281	rBV	114169	176878	16.51%	2.335%

Sum of corrected areas: 7576299

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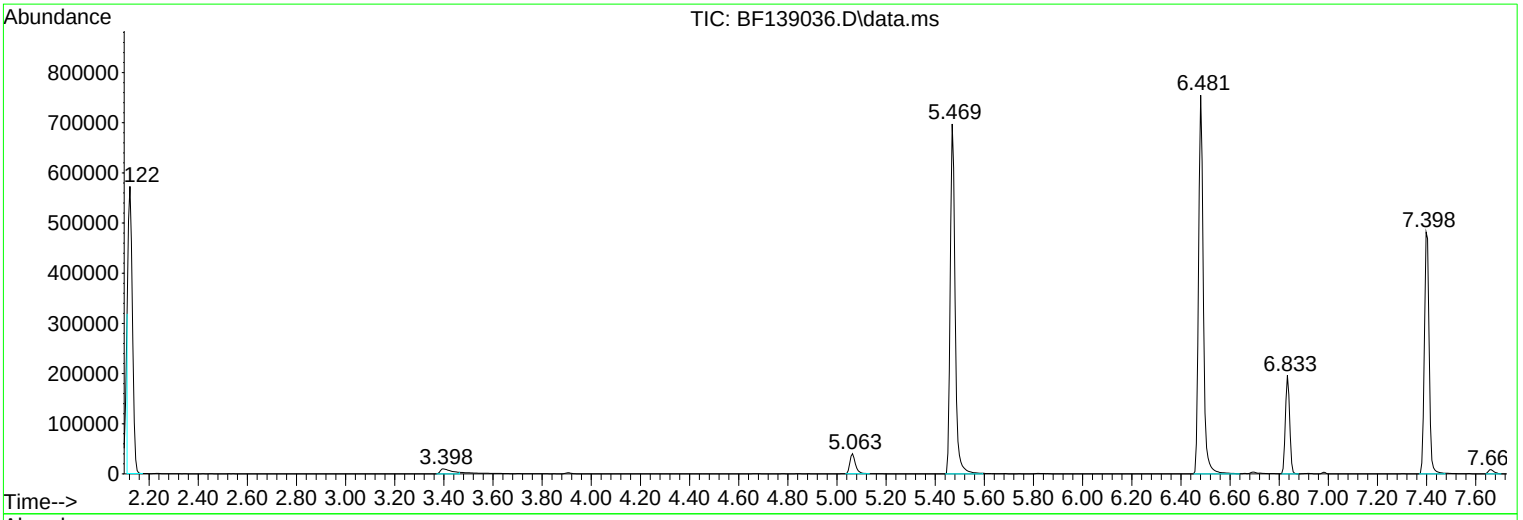
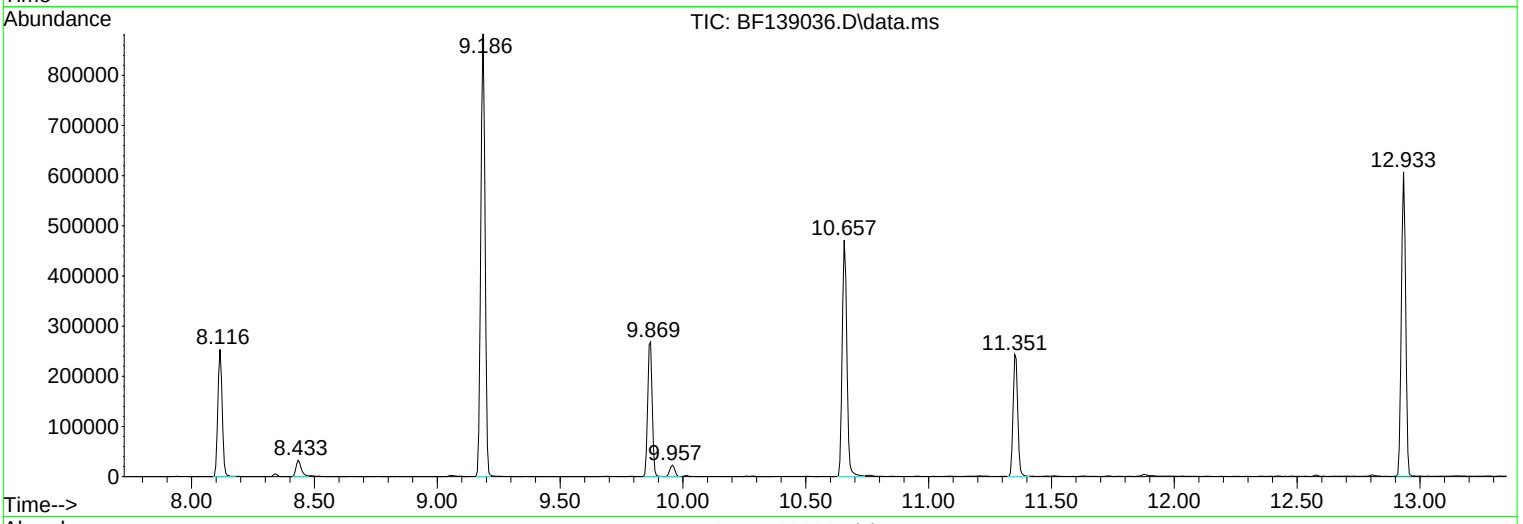
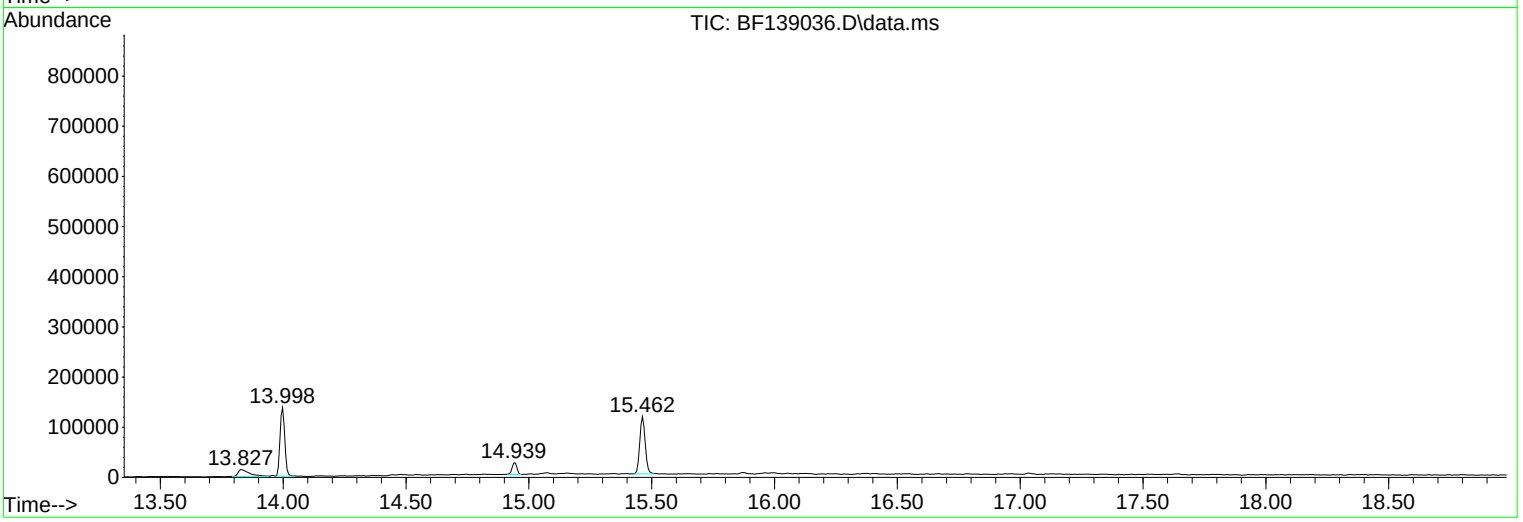
S-856-J-S0-3-3.5-080924

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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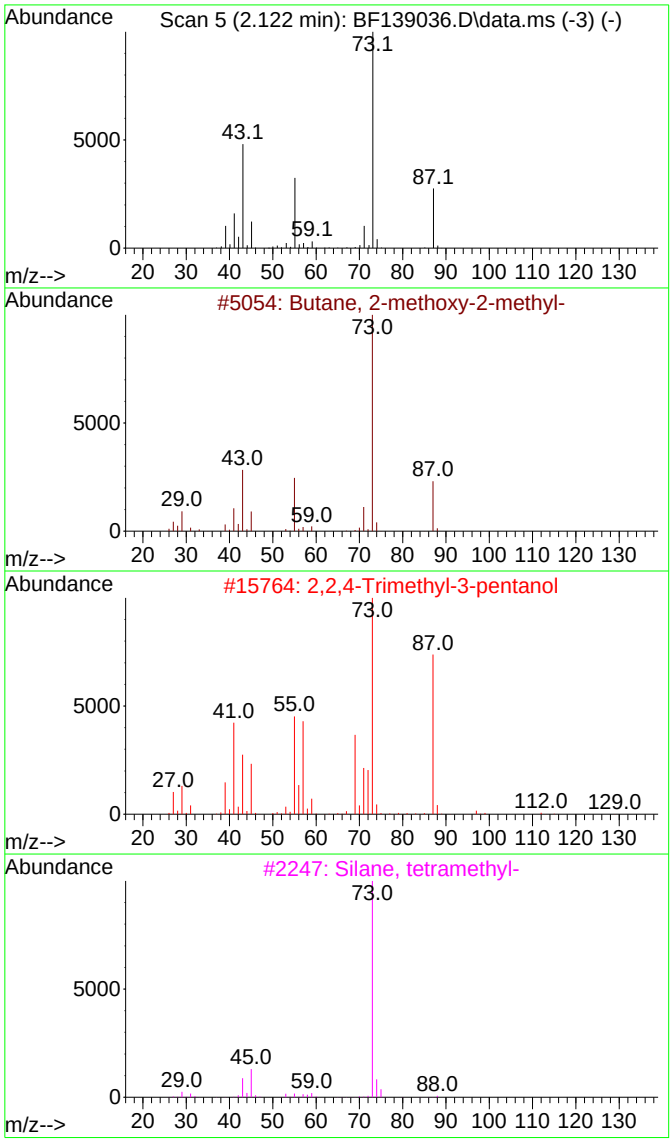
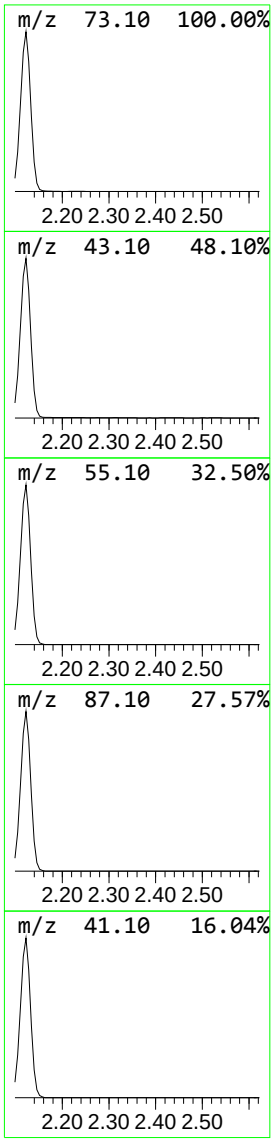
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	57.54 ng	683932	1,4-Dichlorobenzene-d4	6.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Acq On : 15 Aug 2024 22:16
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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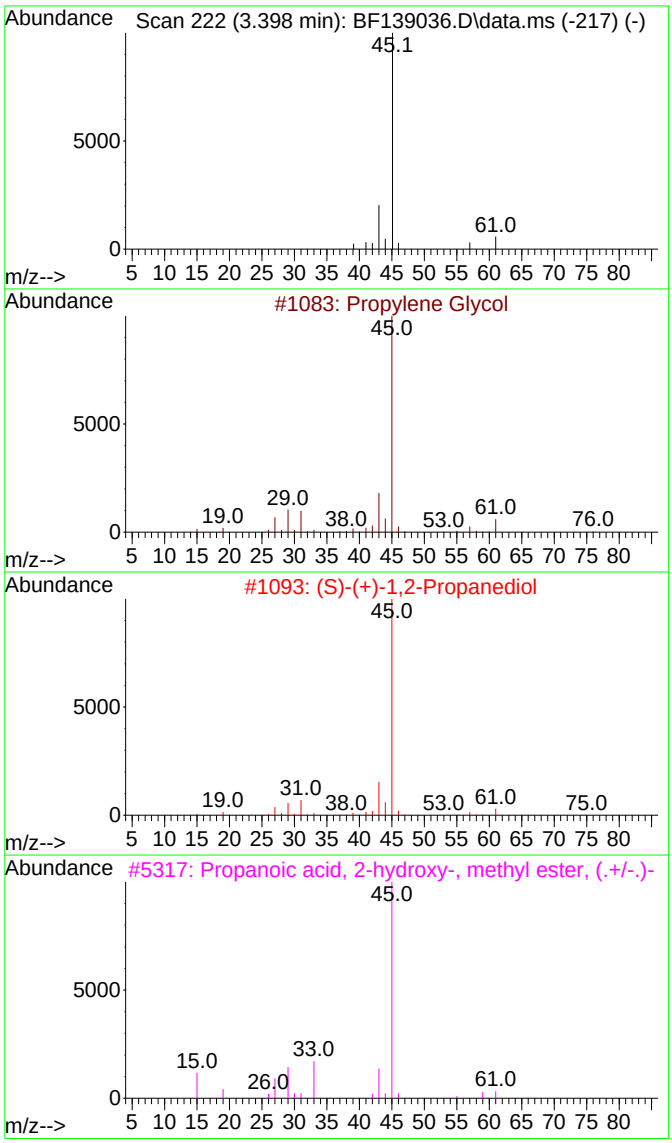
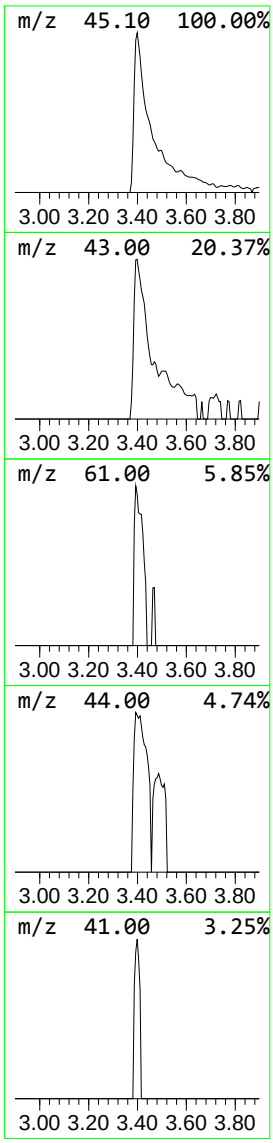
****

Peak Number 2 unknown3.398 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.398	2.69 ng	32003	1,4-Dichlorobenzene-d4	6.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Formamide	45	CH3NO	000075-12-7	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139036.D
Acq On : 15 Aug 2024 22:16
Operator : RC/JU
Sample : P3573-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-856-J-S0-3-3.5-080924

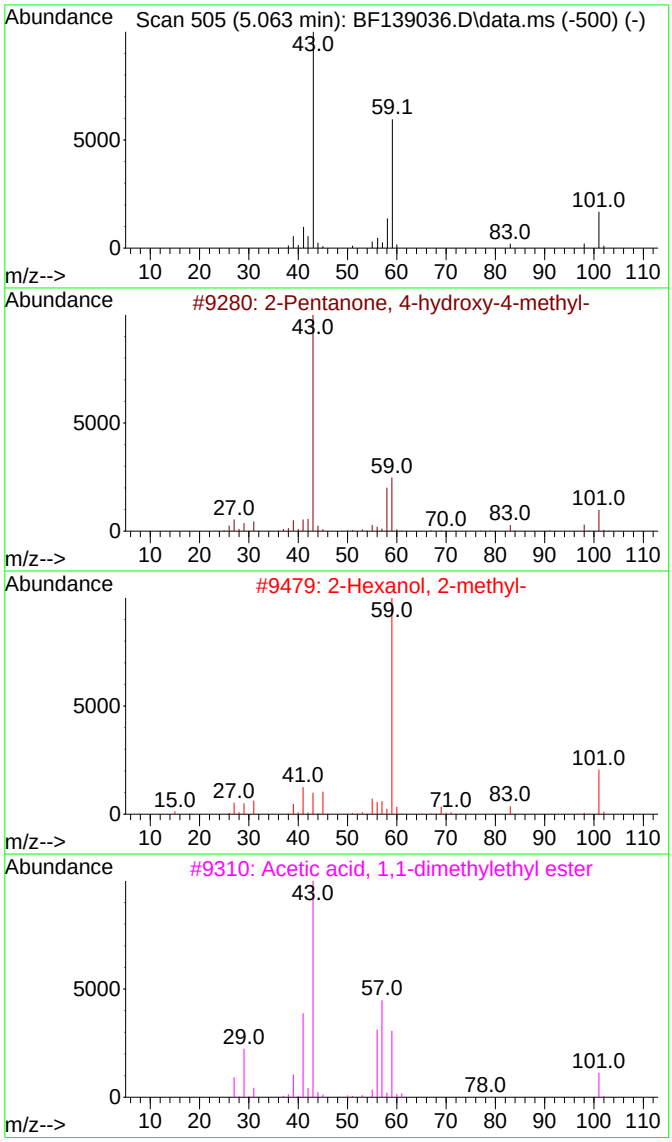
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

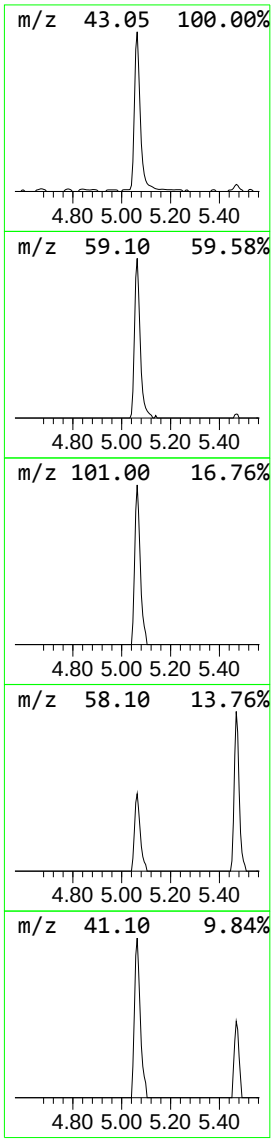
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	5.28 ng	62810	1,4-Dichlorobenzene-d4	6.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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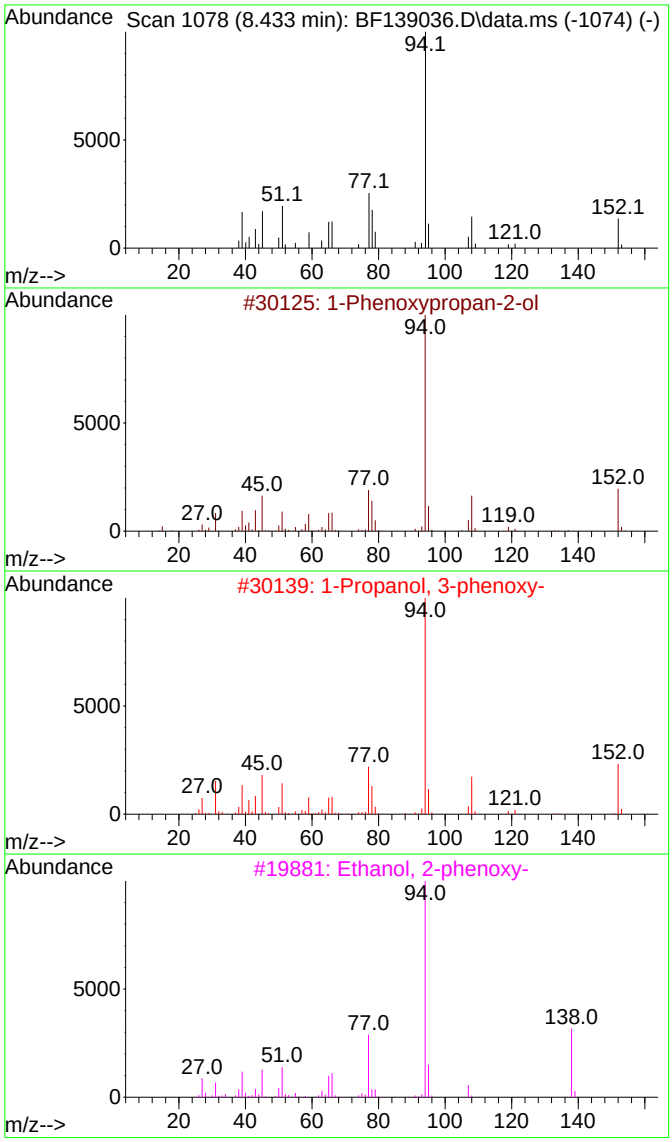
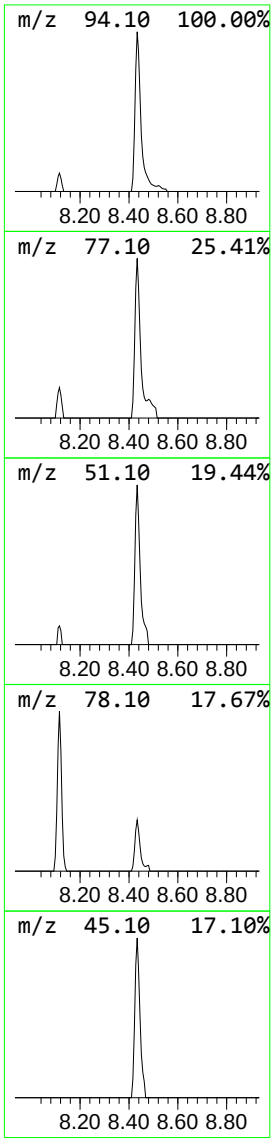
****
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	3.13 ng	49268	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	90
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	59





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
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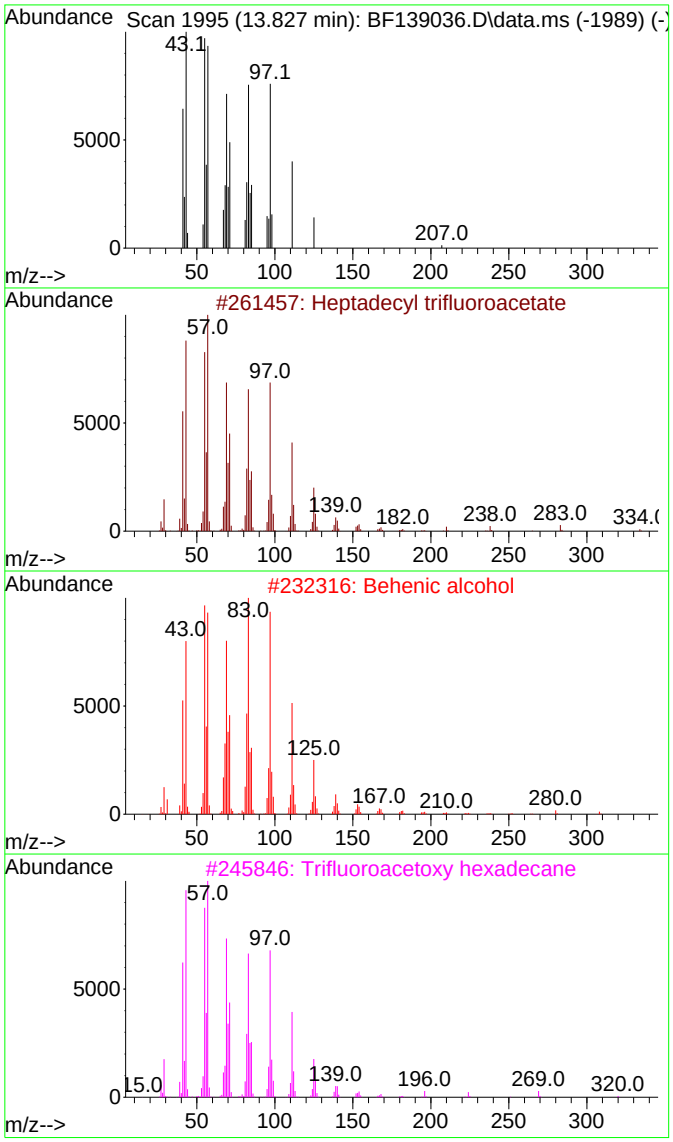
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

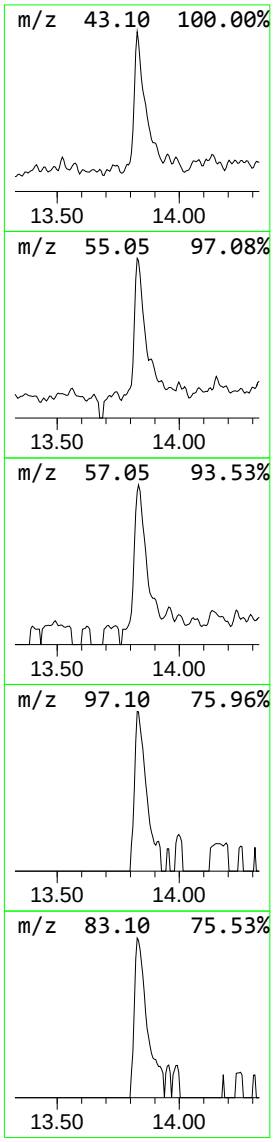
****

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.99 ng	44775	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





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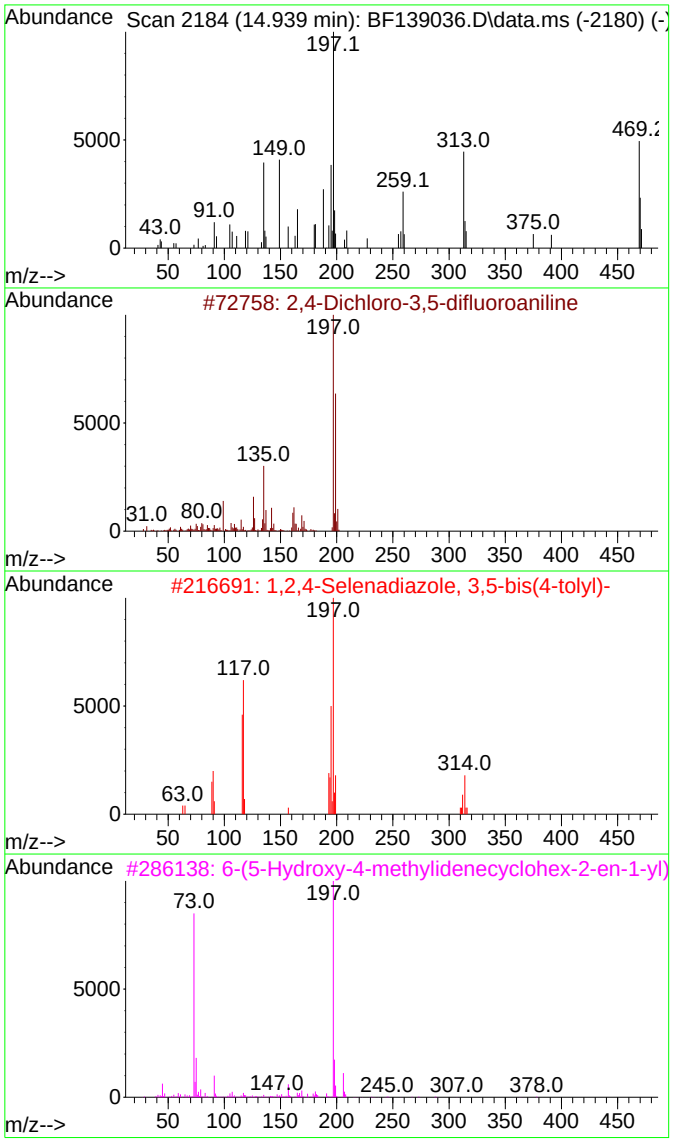
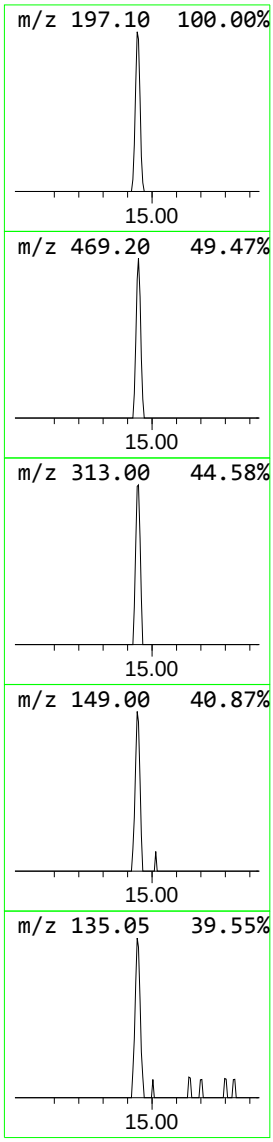
****

Peak Number 6 unknown14.939 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	3.57 ng	31602	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dichloro-3,5-difluoroaniline	197	C6H3Cl2F2N	050408-95-2	12
2	1,2,4-Selenadiazole, 3,5-bis(4-t...	314	C16H14N2Se	068723-60-4	12
3	6-(5-Hydroxy-4-methylidenecycloh...	378	C21H38O2Si2	1000495-91-4	10
4	Tacrine, N-methyl-	212	C14H16N2	1000452-04-1	10
5	Glutaric acid, monoamide, N,N-di...	367	C23H29NO3	1000360-23-2	9





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.122	57.5	ng	683932	1	6.833	237705	20.0
unknown3.398	3.398	2.7	ng	32003	1	6.833	237705	20.0
2-Pentanone, 4-...	5.063	5.3	ng	62810	1	6.833	237705	20.0
1-Phenoxypropan...	8.433	3.1	ng	49268	2	8.116	314473	20.0
Heptadecyl trif...	13.827	5.0	ng	44775	5	13.998	179566	20.0
unknown14.939	14.939	3.6	ng	31602	6	15.462	176878	20.0