LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083121\
Data File : BF125291.D
Acq On : 31 Aug 2021 16:32
Operator : JU/CG
Sample : M3550-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-1

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125291.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.928	137	143	149	rVB	492915	694312	10.47%	1.691%
2	3.798	286	291	296	rBV	60919	80982	1.22%	0.197%
3	4.728	444	449	453	rBV	818086	826507	12.46%	2.013%
4	4.793	456	460	465	rVB	104766	101778	1.53%	0.248%
5	5.157	517	522	527	rBV2	534522	755416	11.39%	1.840%
6	5.545	583	588	591	rBV	4352614	4255797	64.15%	10.365%
7	6.545	753	758	761	rBV	3799825	3807183	57.39%	9.273%
8	6.916	817	821	824	rBV	1212215	1061603	16.00%	2.586%
9	7.481	912	917	920	rBV	3022504	3090312	46.58%	7.527%
10	8.098	1018	1022	1035	rBV	1164855	1743732	26.28%	4.247%
11	8.198	1035	1039	1042	rVB	1588350	1380510	20.81%	3.362%
12	9.269	1217	1221	1232	rBV	5779468	5492301	82.79%	13.377%
13	9.380	1237	1240	1245	rVB	82449	87261	1.32%	0.213%
14	9.951	1333	1337	1348	rVB	1820896	1658138	24.99%	4.039%
15	10.739	1467	1471	1487	rVB	3960836	4031168	60.76%	9.818%
16	11.439	1586	1590	1596	rBV	2116704	1819801	27.43%	4.432%
17	11.821	1651	1655	1659	rBV	259422	203305	3.06%	0.495%
18	11.957	1674	1678	1682	rBV	69855	86484	1.30%	0.211%
19	12.527	1772	1775	1778	rVB	362364	272967	4.11%	0.665%
20	12.616	1786	1790	1793	rVB	102388	88429	1.33%	0.215%
21	13.027	1855	1860	1863	rBV	6826764	6634164	100.00%	16.158%
22	13.951	2013	2017	2027	rBV2	96842	202156	3.05%	0.492%
23	14.080	2035	2039	2051	rVB	1531537	1448021	21.83%	3.527%
24	15.580	2289	2294	2305	rBV	833242	1235112	18.62%	3.008%

Sum of corrected areas: 41057439

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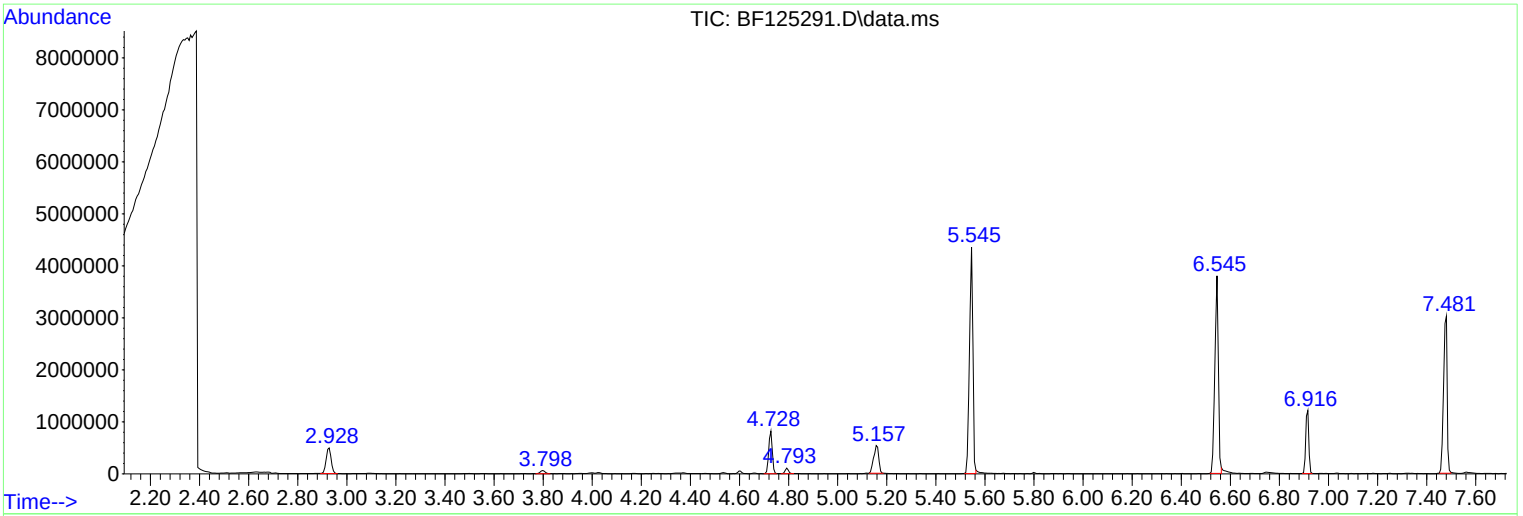
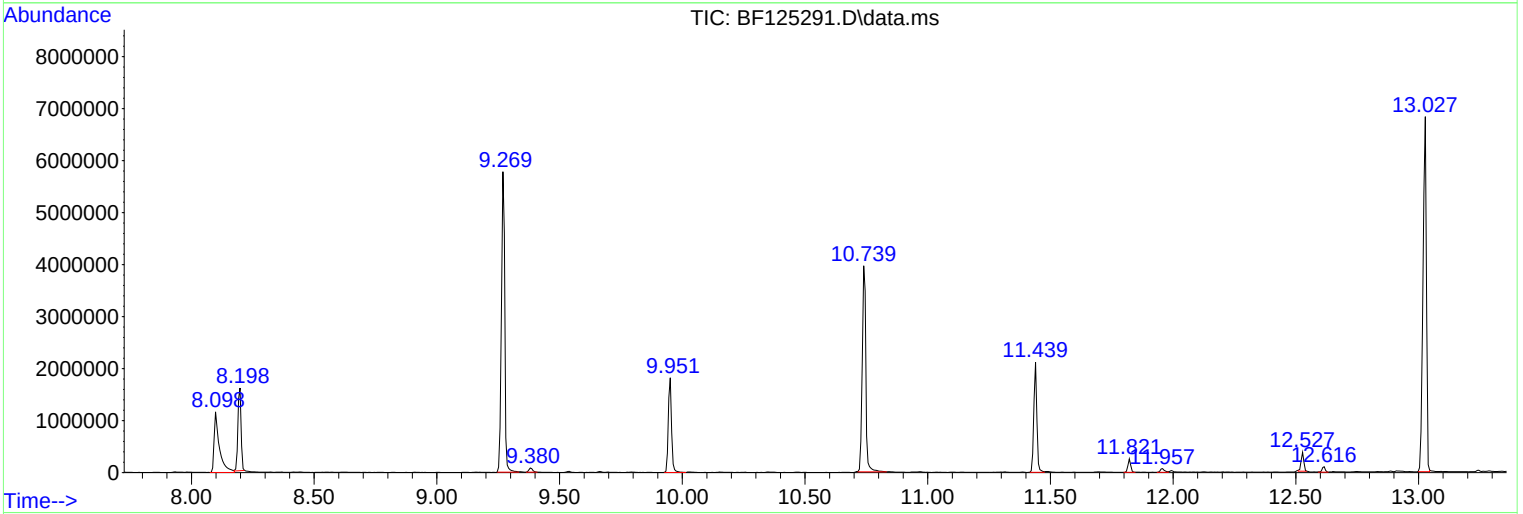
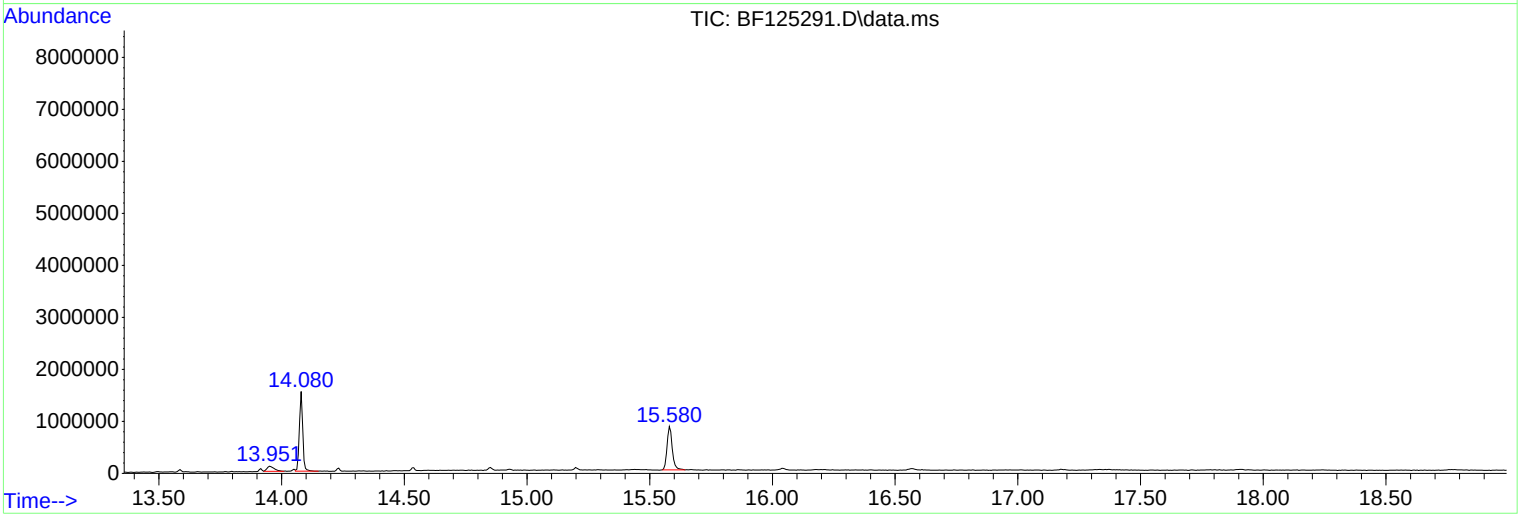
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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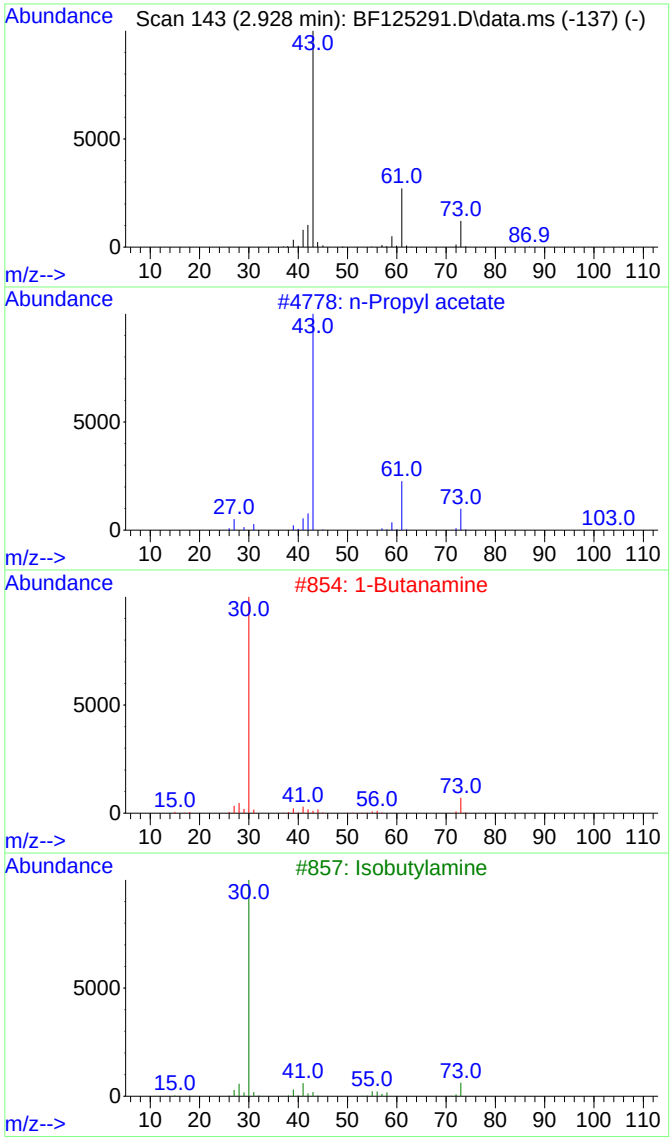
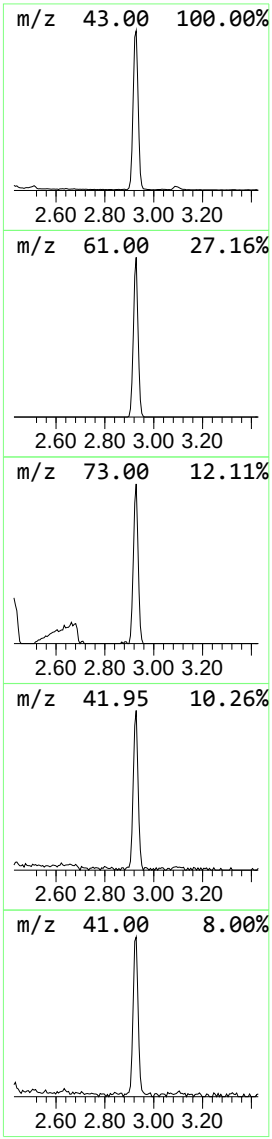
****

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.928	13.08 ng	694312	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	Hydrogen azide	43	HN3	007782-79-8	4
5	Acetic acid, 2-fluoroethyl ester	106	C4H7FO2	1000367-87-9	4





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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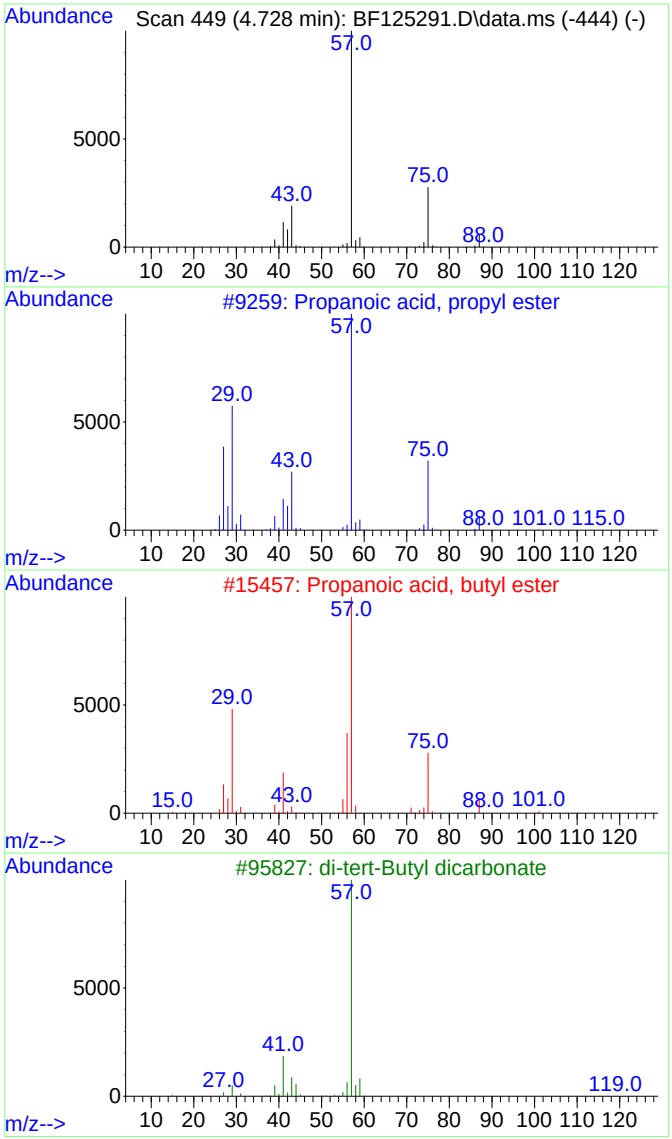
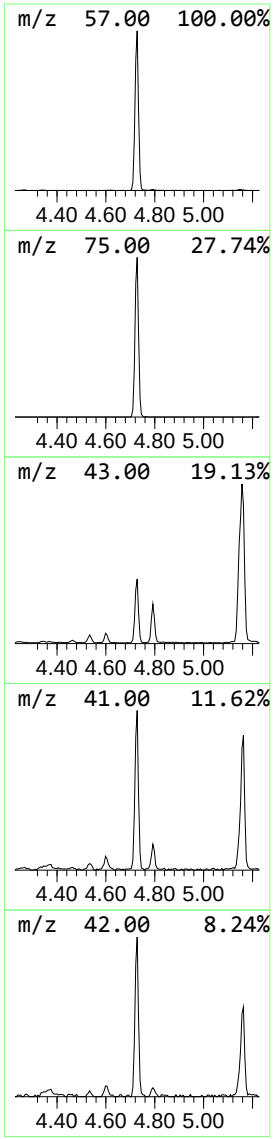
****
Peak Number 2 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.728	15.57 ng	826507	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5	Neopentylamine	87	C5H13N	005813-64-9	4





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Sample : M3550-01
Misc :
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Instrument : BNA_F
ClientSampleId : WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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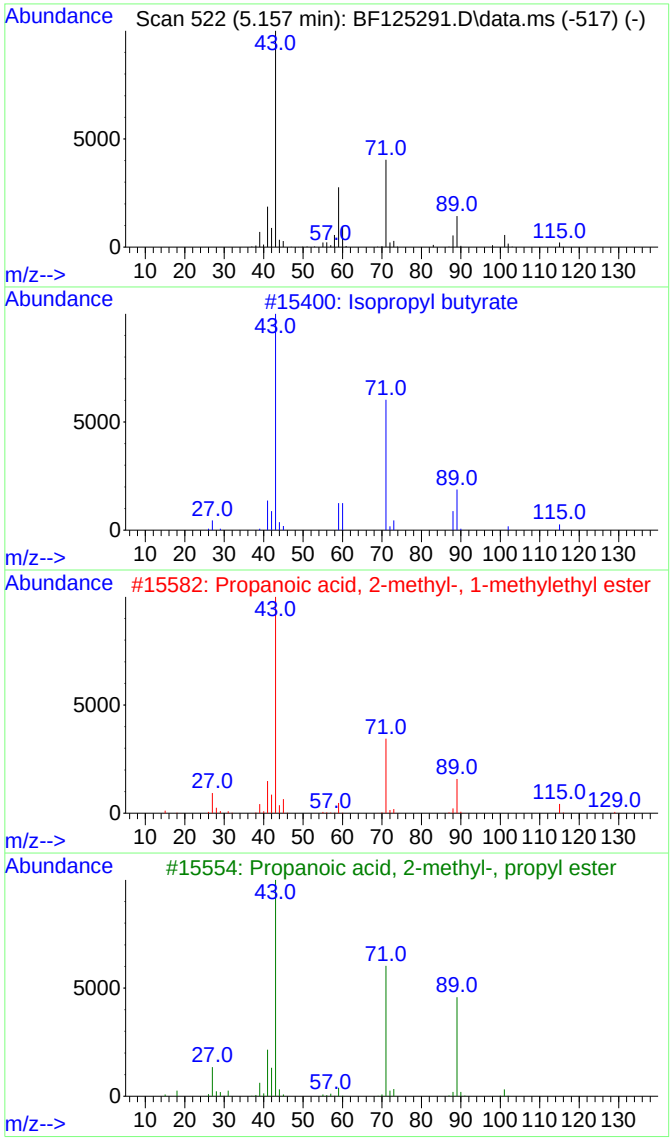
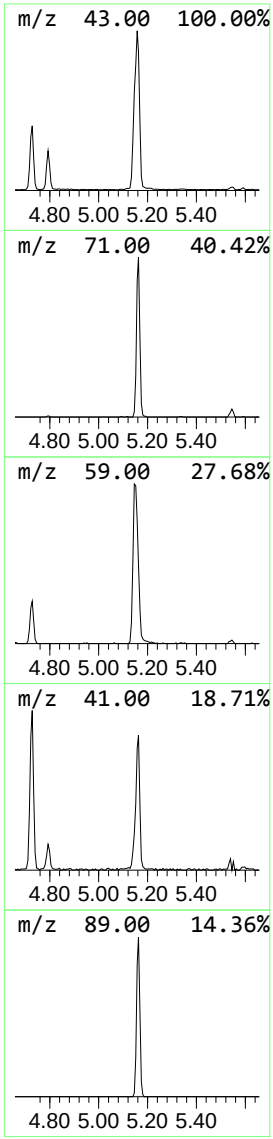
Peak Number 3 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	14.23 ng	755416	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	59
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	53
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	50
4	Butanoic acid, 2-ethyl-, methyl ...	130	C7H14O2	000816-11-5	36
5	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	32





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Instrument : BNA_F
ClientSampleId : WC-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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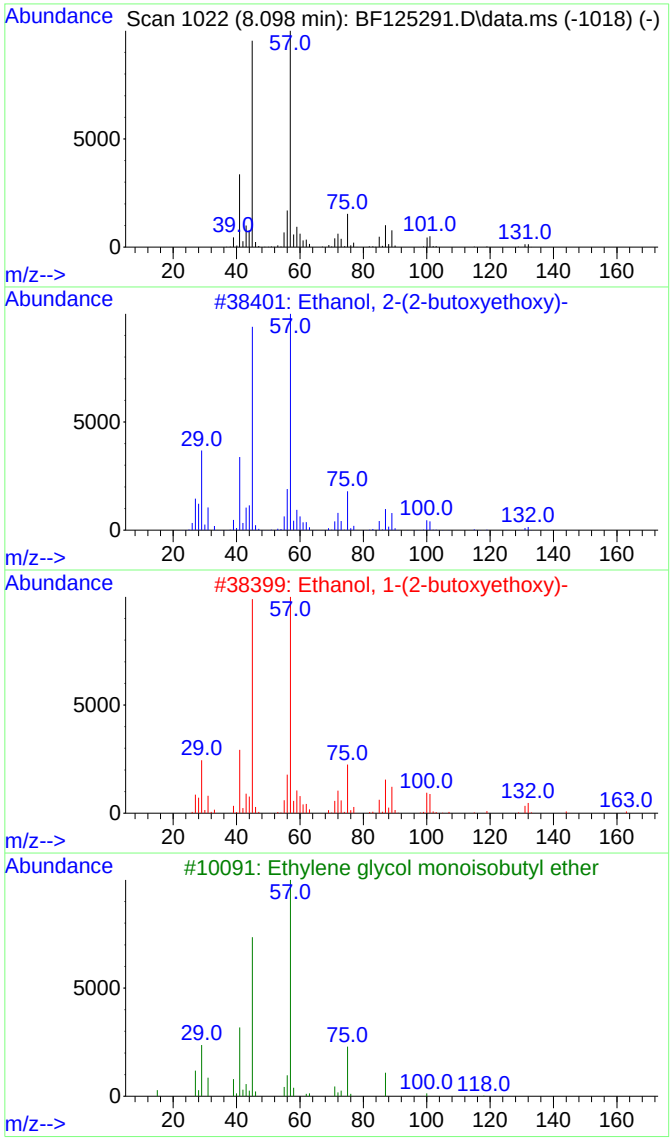
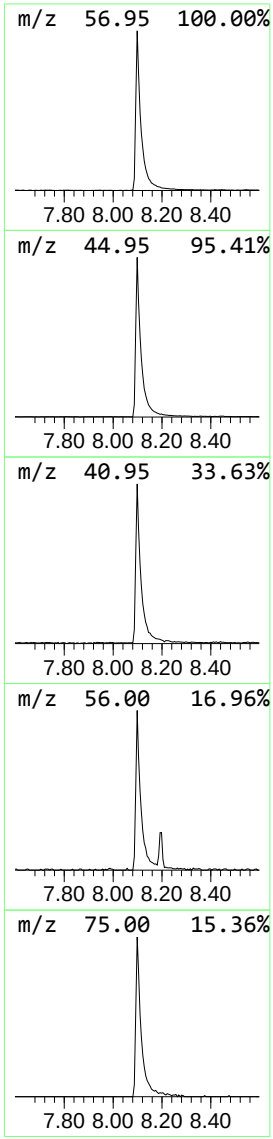
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	25.26 ng	1743730	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





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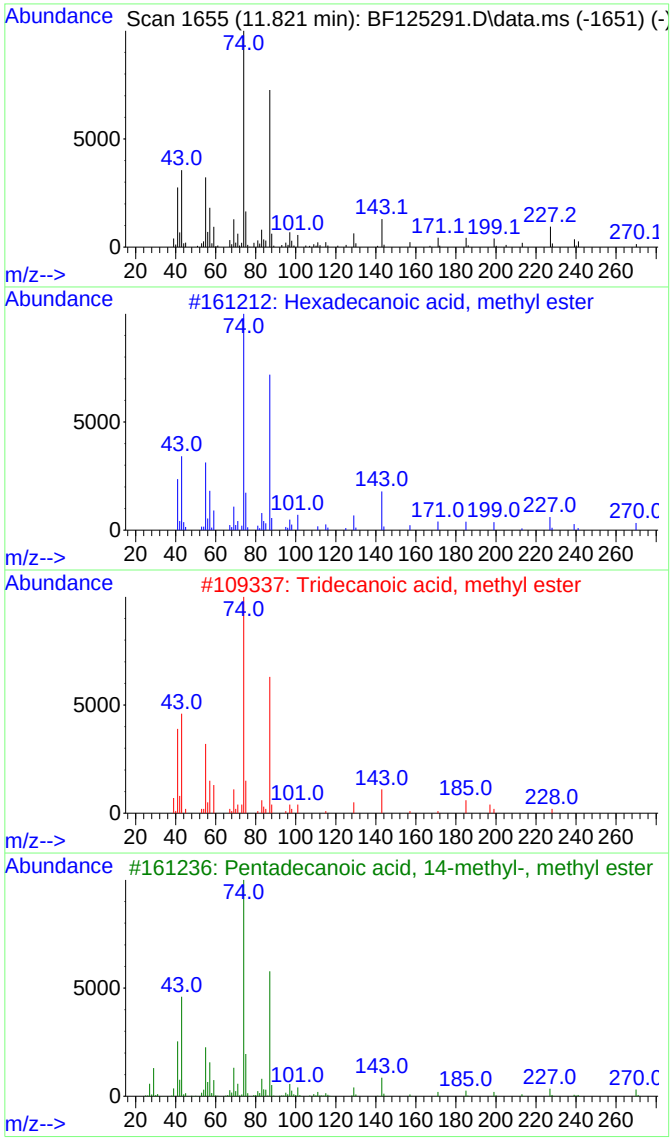
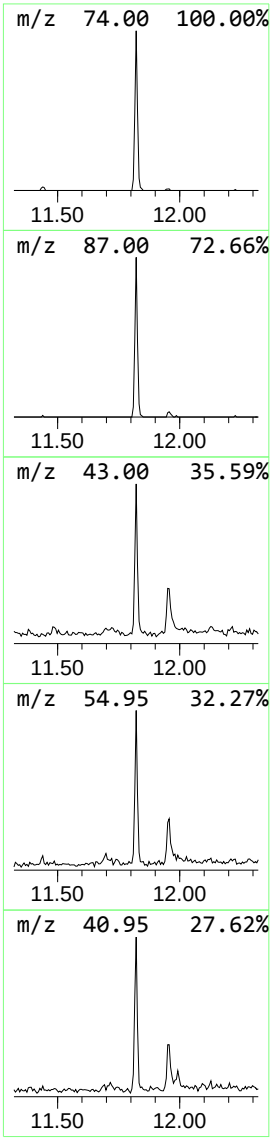
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	2.23 ng	203305	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	89
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83





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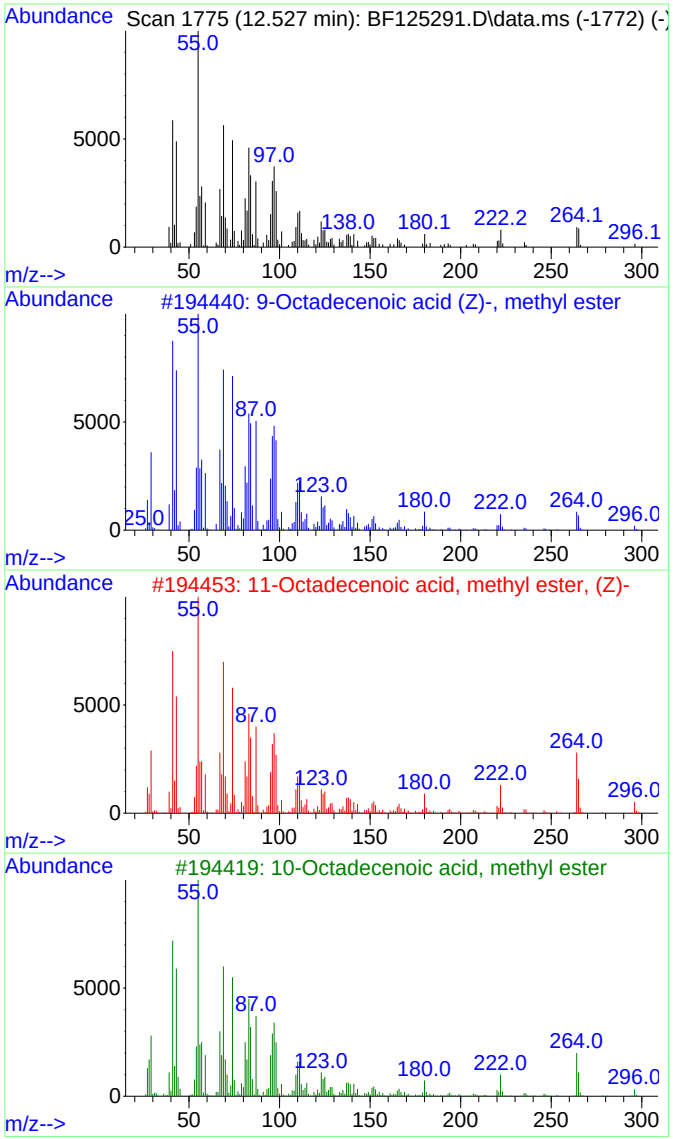
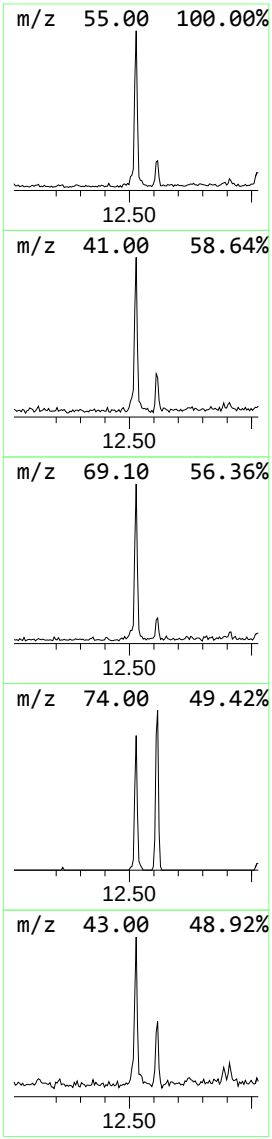
****
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	3.00 ng	272967	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99





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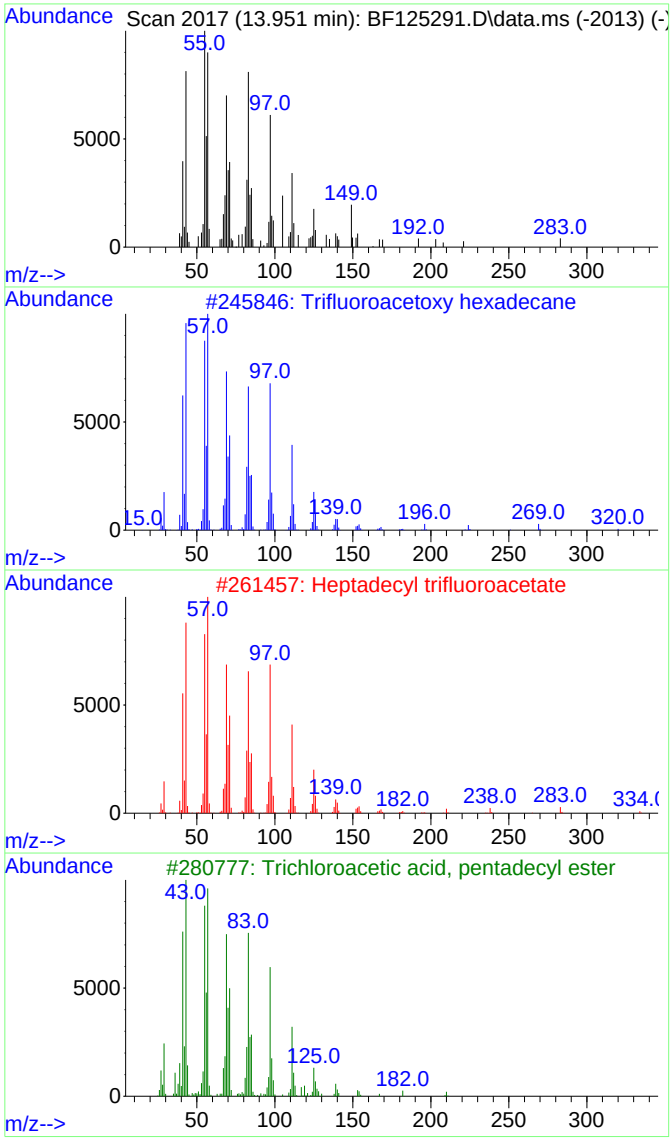
TIC Integration Parameters: LSCINT.P

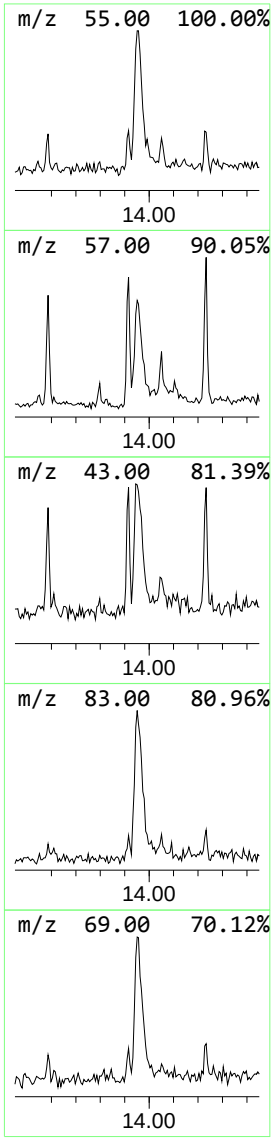
****

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	2.79 ng	202156	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	92
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	90





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.928	13.1	ng	694312	1	6.916	1061600	20.0
Propanoic acid,...	4.728	15.6	ng	826507	1	6.916	1061600	20.0
Isopropyl butyrate	5.157	14.2	ng	755416	1	6.916	1061600	20.0
Ethanol, 2-(2-b...	8.098	25.3	ng	1743730	2	8.198	1380510	20.0
Hexadecanoic ac...	11.822	2.2	ng	203305	4	11.439	1819800	20.0
9-Octadecenoic ...	12.527	3.0	ng	272967	4	11.439	1819800	20.0
Trifluoroacetox...	13.951	2.8	ng	202156	5	14.080	1448020	20.0