LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
Data File : BF125424.D
Acq On : 10 Sep 2021 15:12
Operator : JU/CG
Sample : M3692-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WM-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: BF125424.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	9	15	27	rVB	888630	1203382	46.07%	5.114%
2	2.287	30	34	39	rVB	36704	44328	1.70%	0.188%
3	5.104	509	513	525	rVB	101694	133242	5.10%	0.566%
4	5.510	578	582	585	rBV	2864070	2525563	96.68%	10.733%
5	6.516	748	753	756	rBV	2573964	2486440	95.18%	10.567%
6	6.886	812	816	819	rBV	972635	836939	32.04%	3.557%
7	7.445	906	911	914	rBV	1789437	1649085	63.13%	7.008%
8	8.069	1013	1017	1030	rBV	459000	653610	25.02%	2.778%
9	8.169	1030	1034	1037	rVB	1228178	1070838	40.99%	4.551%
10	9.239	1212	1216	1228	rBV	2684430	2612234	100.00%	11.101%
11	9.580	1270	1274	1277	rVB	39778	35049	1.34%	0.149%
12	9.922	1328	1332	1344	rBV	1247177	1221138	46.75%	5.190%
13	10.716	1463	1467	1483	rVB	2022850	1893342	72.48%	8.046%
14	11.410	1582	1585	1589	rBV	1305904	1265482	48.44%	5.378%
15	11.798	1648	1651	1654	rVB	68586	50870	1.95%	0.216%
16	11.933	1670	1674	1685	rBV	384072	407956	15.62%	1.734%
17	12.715	1804	1807	1818	rBV	172244	198116	7.58%	0.842%
18	12.998	1851	1855	1858	rBV	3144051	2607960	99.84%	11.083%
19	13.757	1981	1984	1989	rBV	142889	137488	5.26%	0.584%
20	13.886	2002	2006	2008	rBV2	30039	32460	1.24%	0.138%
21	13.921	2008	2012	2026	rVV3	124037	284941	10.91%	1.211%
22	14.057	2031	2035	2039	rBV	1262635	1058749	40.53%	4.499%
23	14.821	2160	2165	2170	rVB5	29705	50804	1.94%	0.216%
24	15.168	2221	2224	2230	rVB	50711	57931	2.22%	0.246%
25	15.551	2283	2289	2295	rBV	695497	953760	36.51%	4.053%
26	15.998	2361	2365	2371	rVB2	41597	58966	2.26%	0.251%

Sum of corrected areas: 23530673

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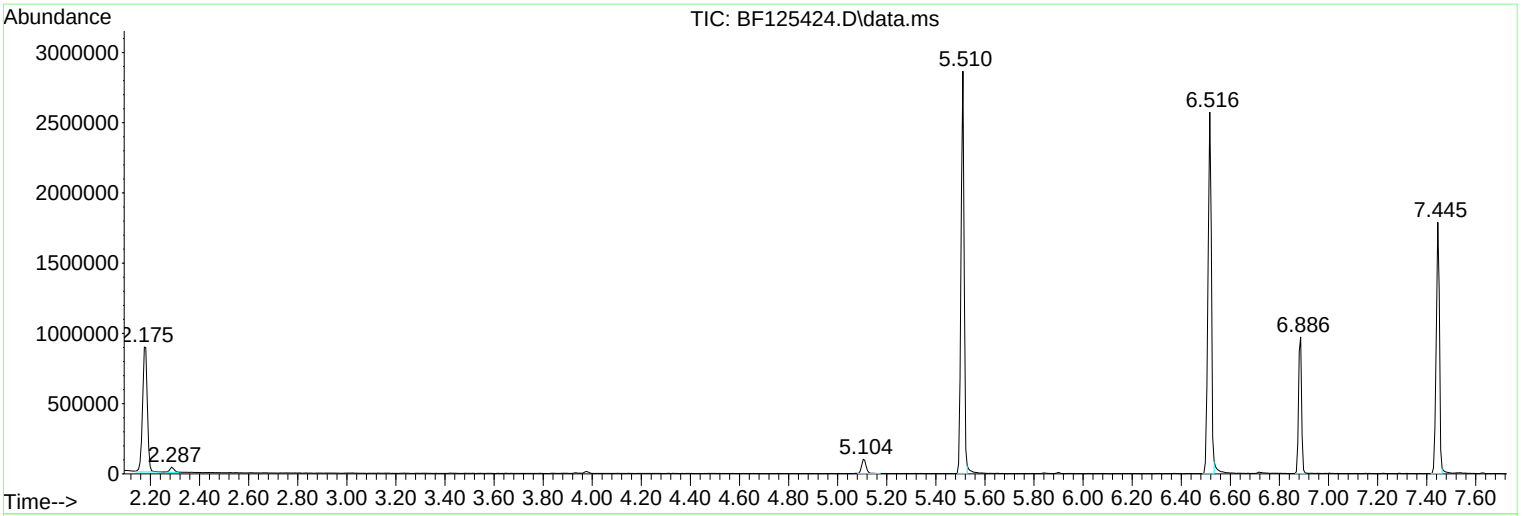
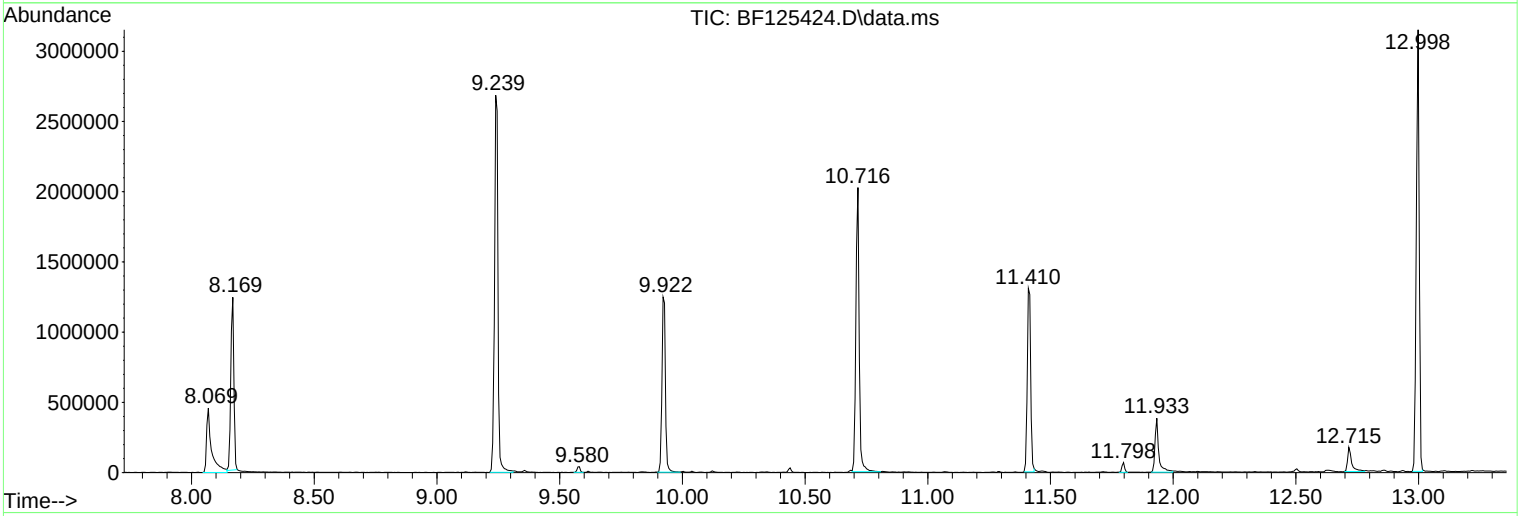
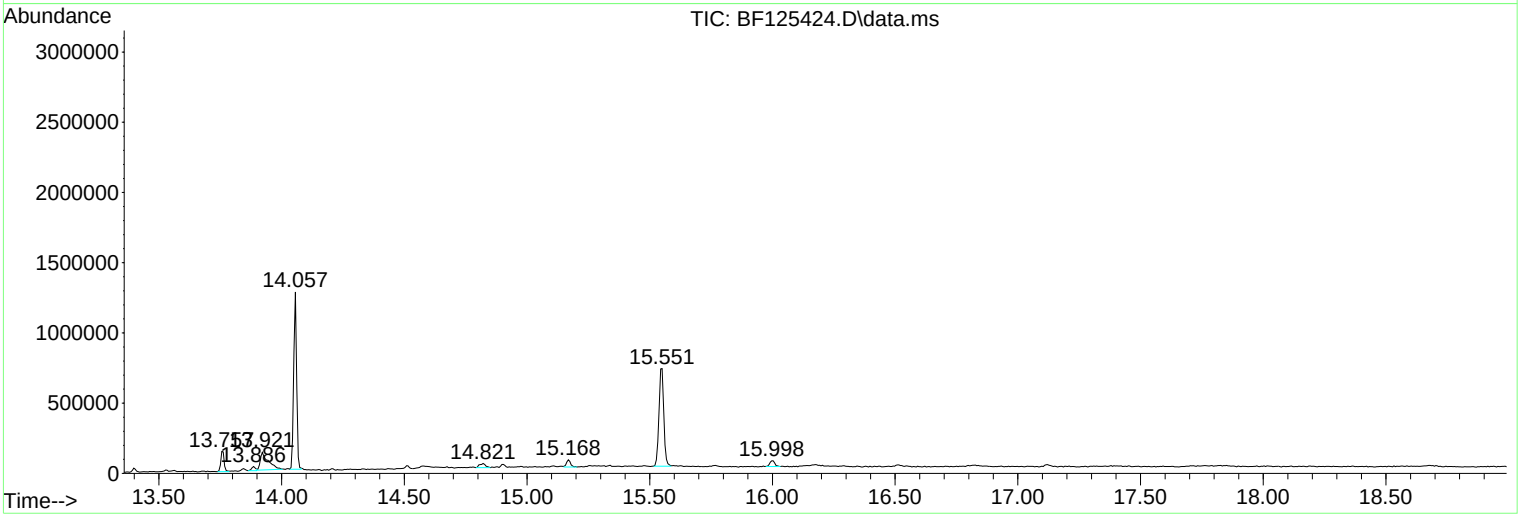
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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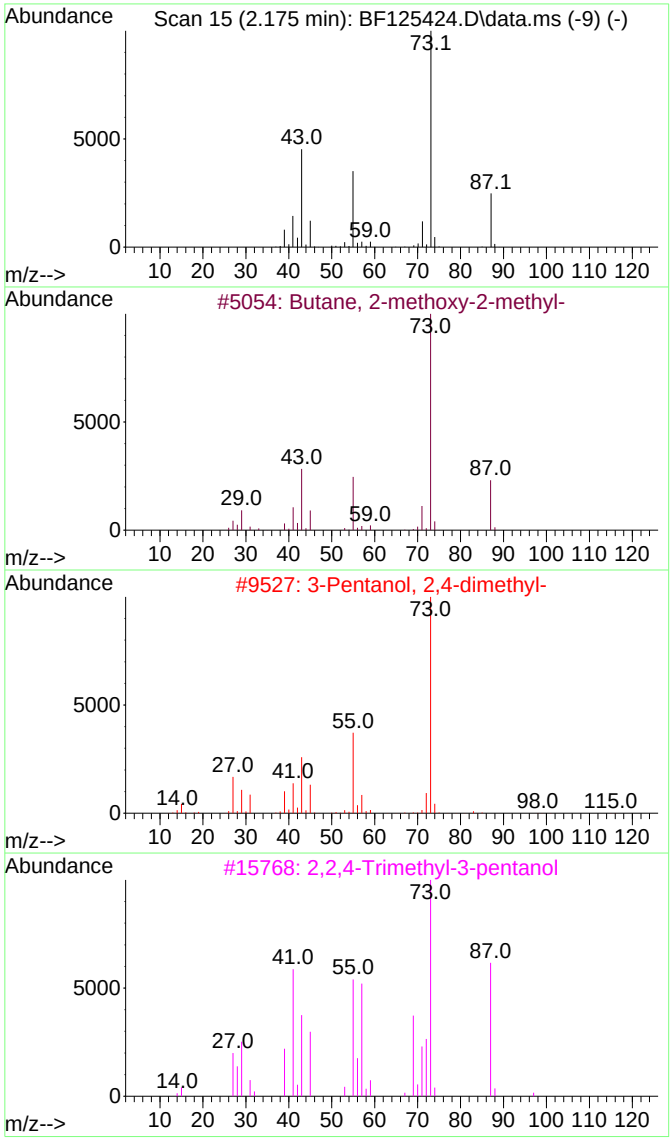
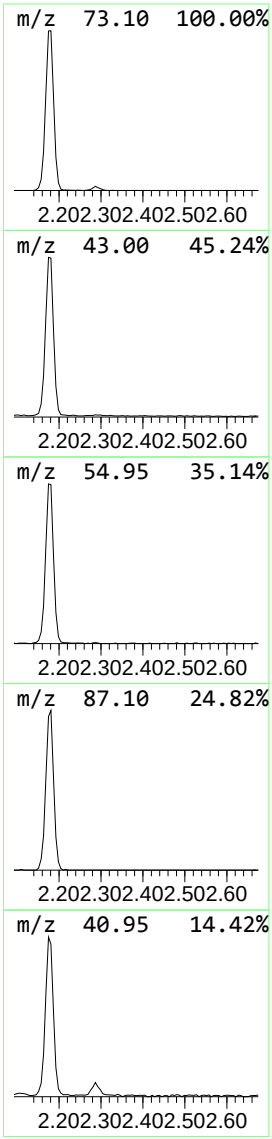
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	28.76 ng	1203380	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28





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Data File : BF125424.D
Acq On : 10 Sep 2021 15:12
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ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WM-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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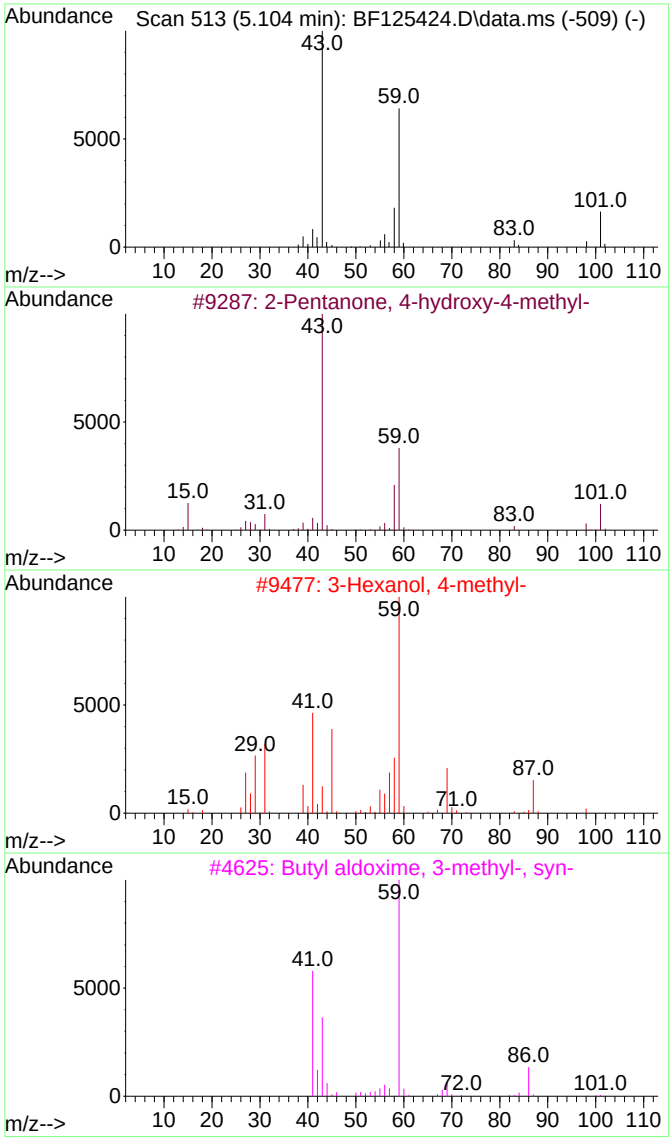
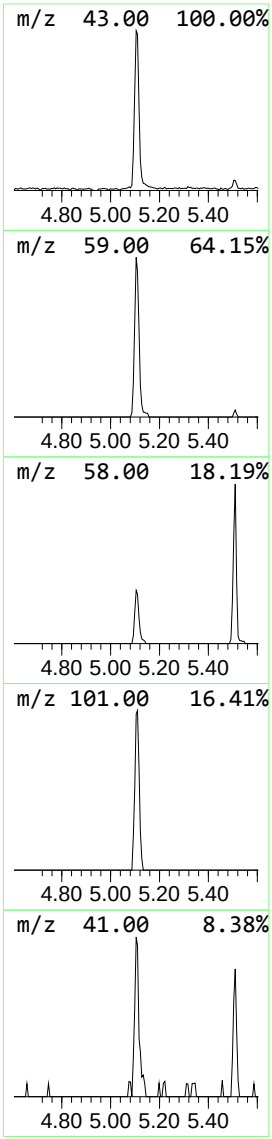
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.18 ng	133242	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Sample : M3692-01
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Instrument : BNA_F
ClientSampleId : WM-1

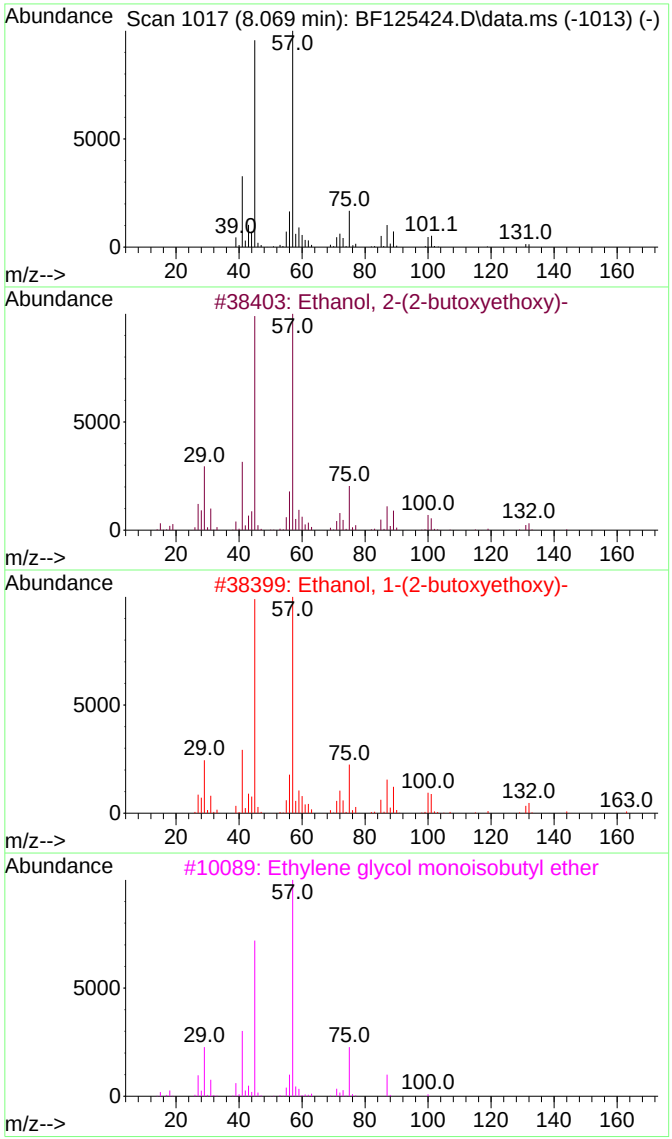
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

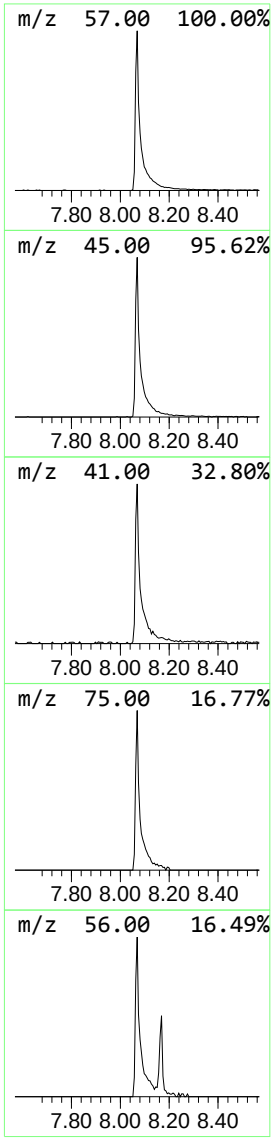
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	12.21 ng	653610	Naphthalene-d8	8.169

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	64
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56





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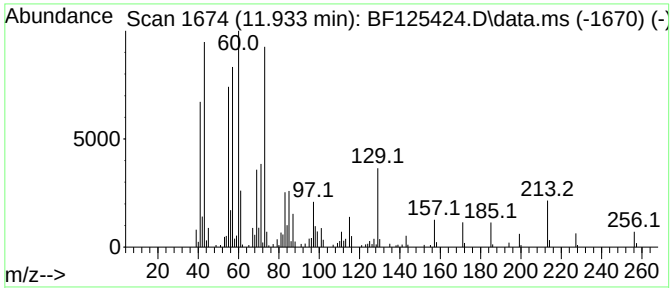
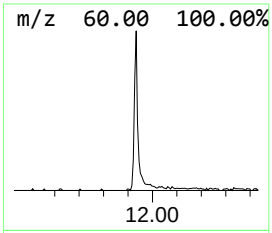
****

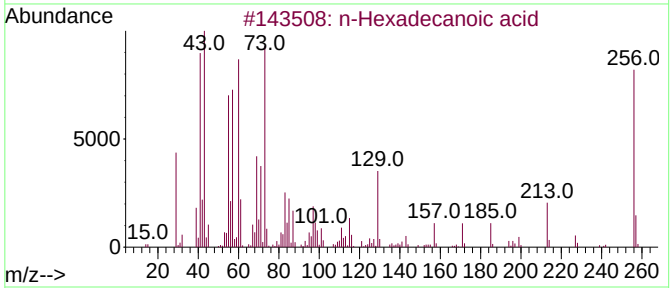
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

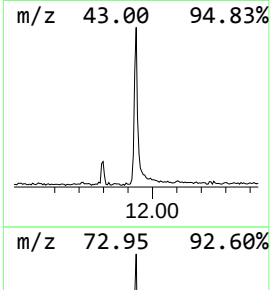
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	6.45 ng	407956	Phenanthrene-d10	11.410

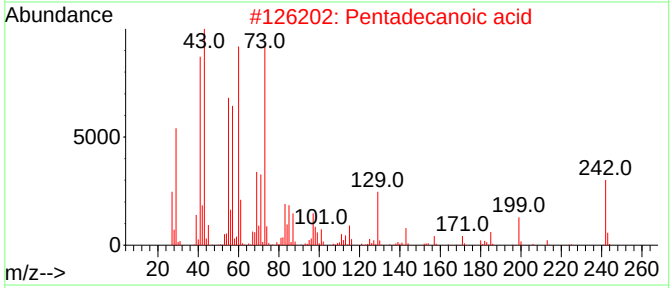
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55

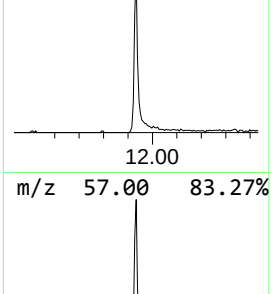


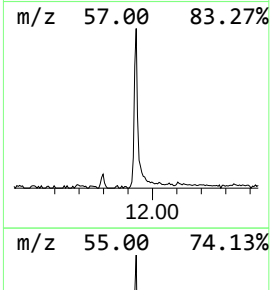


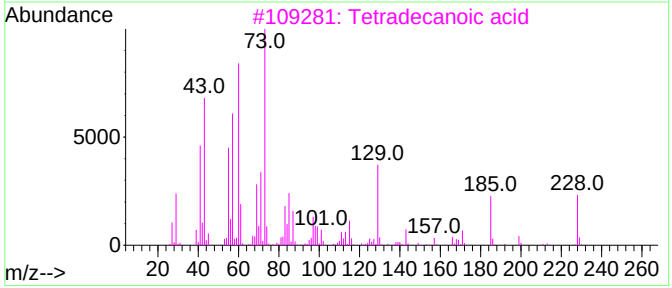


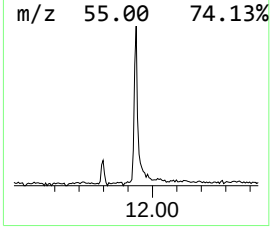












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

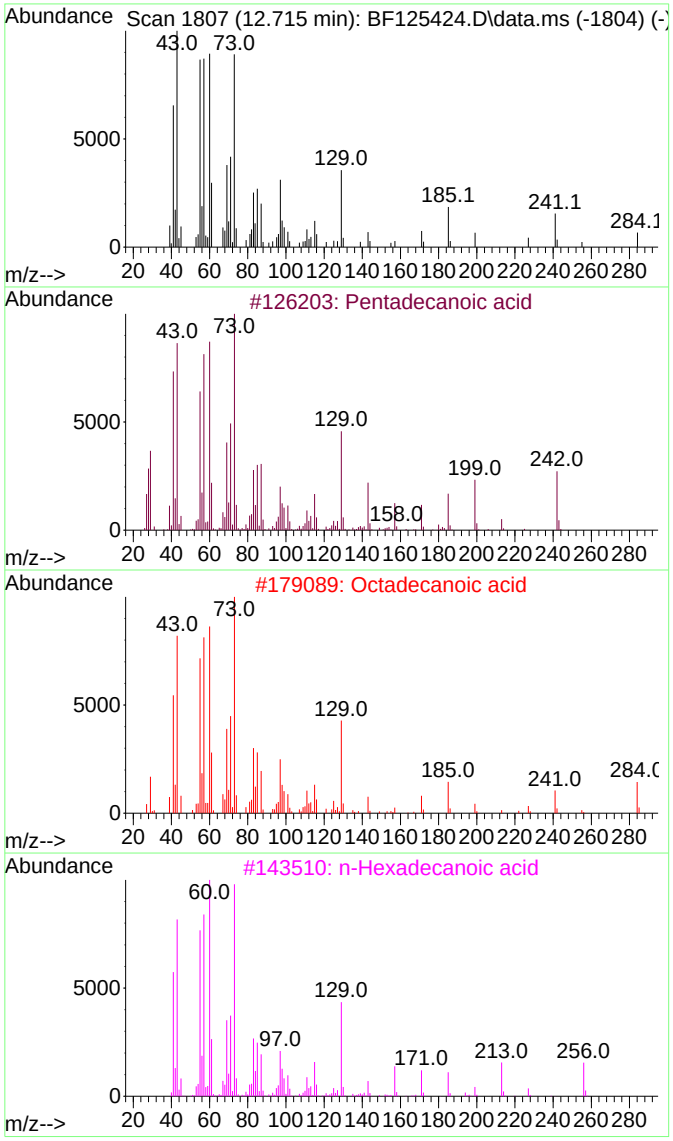
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

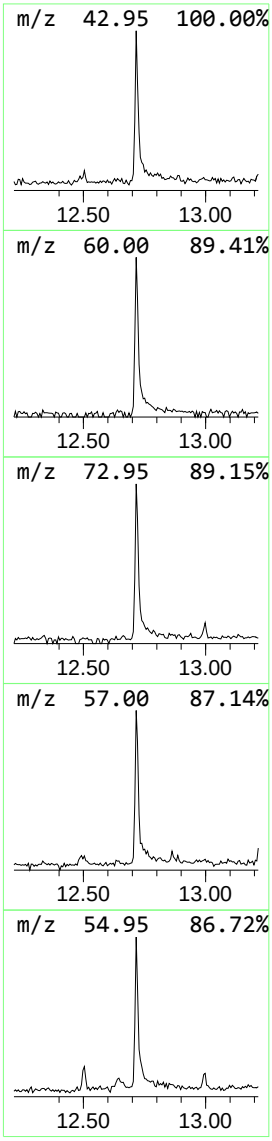
****

Peak Number 5 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	3.13 ng	198116	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	Octadecanoic acid	284	C18H36O2	000057-11-4	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Undecanoic acid	186	C11H22O2	000112-37-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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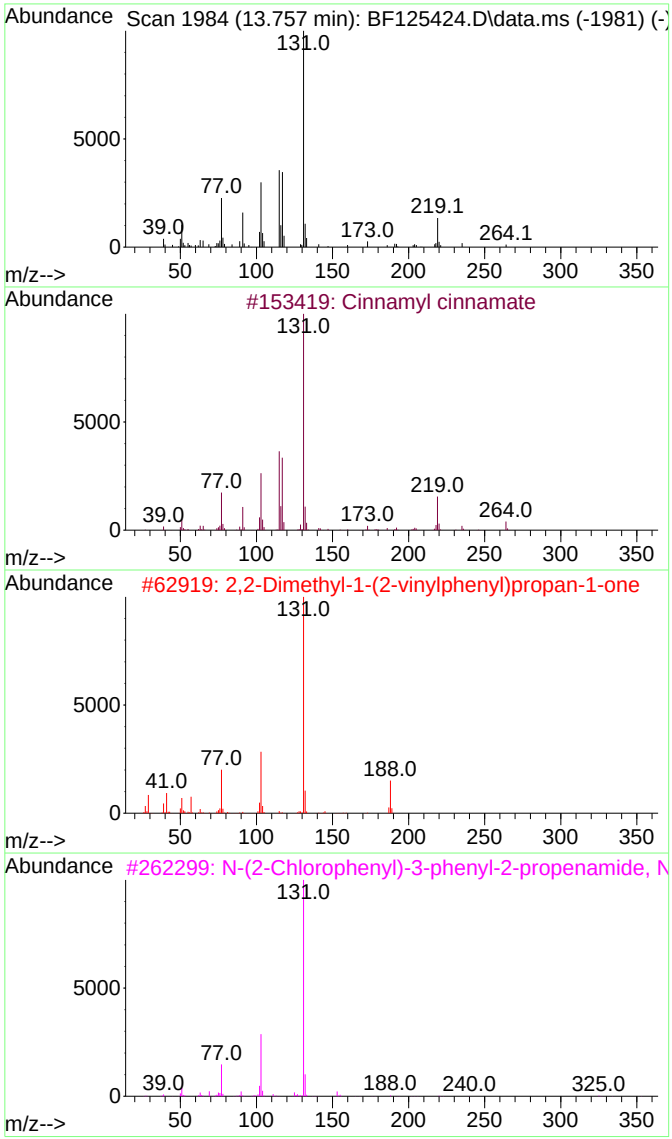
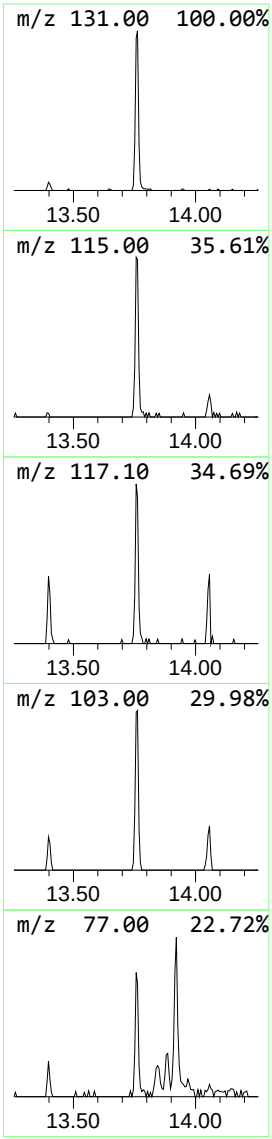
****

Peak Number 6 Cinnamyl cinnamate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	2.60 ng	137488	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	90
2	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
3	N-(2-Chlorophenyl)-3-phenyl-2-pr...	353	C17H11ClF3NO2	1000492-36-9	50
4	1-(4-Ethynylphenyl)-2-methylprop...	174	C12H14O	1000466-39-4	50
5	3-phenylprop-2-enoic anhydride	278	C18H14O3	1010401-87-5	50





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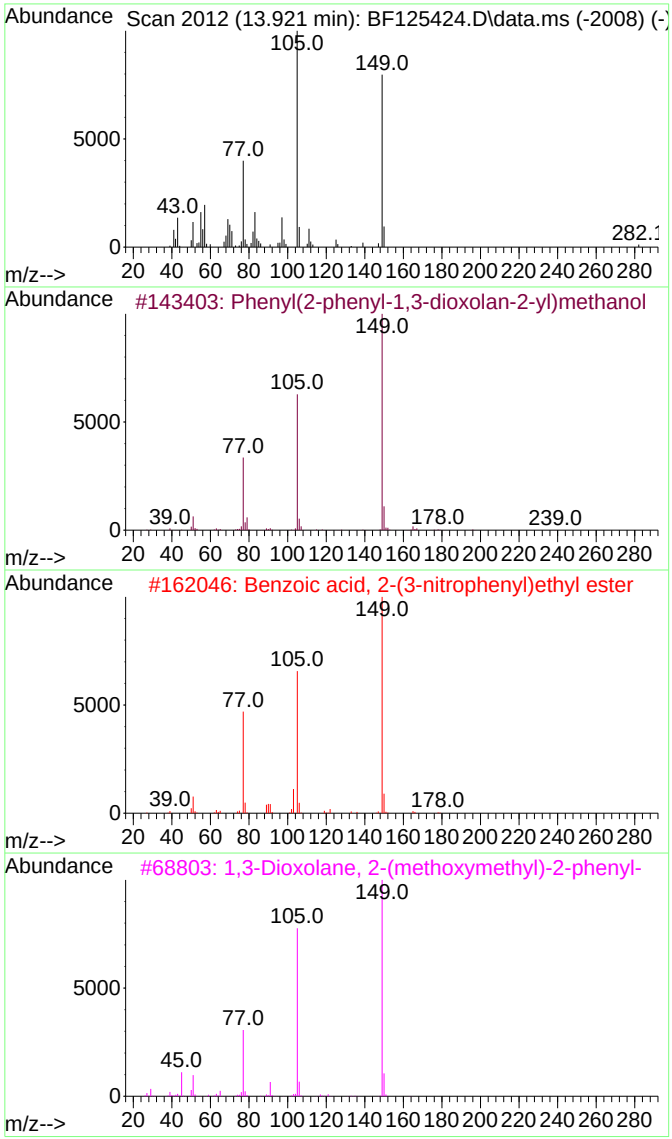
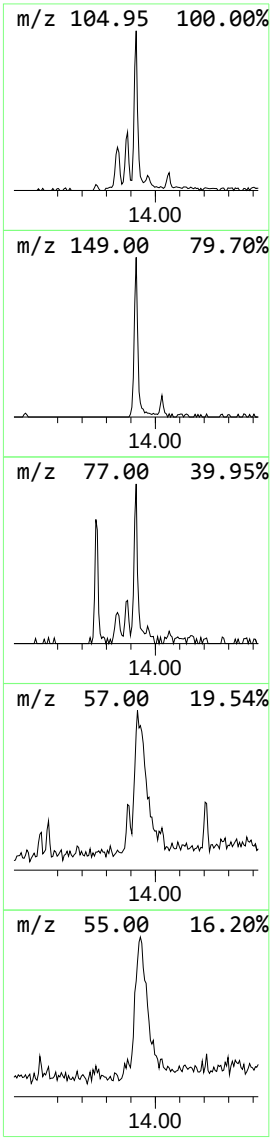
****

Peak Number 7 Phenyl(2-phenyl-1,3-dioxola... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	5.38 ng	284941	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	72
2	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
5	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	53





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST20.L
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.175	28.8	ng	1203380	1	6.886	836939	20.0
2-Pentanone, 4-...	5.104	3.2	ng	133242	1	6.886	836939	20.0
Ethanol, 2-(2-b...	8.069	12.2	ng	653610	2	8.169	1070840	20.0
n-Hexadecanoic ...	11.933	6.5	ng	407956	4	11.410	1265480	20.0
Pentadecanoic acid	12.716	3.1	ng	198116	4	11.410	1265480	20.0
Cinnamyl cinnamate	13.757	2.6	ng	137488	5	14.057	1058750	20.0
Phenyl(2-phenyl...	13.921	5.4	ng	284941	5	14.057	1058750	20.0