LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022122\
Data File : BF126994.D
Acq On : 22 Feb 2022 01:00
Operator : CG\JU
Sample : N1602-07
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220083-AMENDED-BERKELEY-3-COMP

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126994.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.146	482	486	494	rVB	162484	200096	6.31%	1.085%
2	5.540	548	553	556	rBV	2409211	2197951	69.32%	11.922%
3	6.451	704	708	714	rBV	80547	87553	2.76%	0.475%
4	6.540	717	723	726	rBV	2526454	2821159	88.97%	15.302%
5	6.916	783	787	790	rBV	652791	502716	15.85%	2.727%
6	7.481	877	883	886	rBV	1929487	1890175	59.61%	10.253%
7	7.640	906	910	915	rVB2	52801	61899	1.95%	0.336%
8	8.087	983	986	997	rBV	183322	183612	5.79%	0.996%
9	8.198	1000	1005	1008	rBV	774494	685167	21.61%	3.716%
10	8.328	1024	1027	1035	rBV	84785	90767	2.86%	0.492%
11	9.275	1182	1188	1191	rBV	3680183	3170882	100.00%	17.199%
12	9.351	1195	1201	1203	rBV2	32755	38872	1.23%	0.211%
13	9.951	1300	1303	1307	rVB	877058	749032	23.62%	4.063%
14	10.739	1434	1437	1441	rBV	1270842	1191428	37.57%	6.462%
15	10.875	1457	1460	1465	rVB	79692	70444	2.22%	0.382%
16	11.316	1533	1535	1541	rVB2	58875	60254	1.90%	0.327%
17	11.445	1553	1557	1560	rBV	911203	769452	24.27%	4.174%
18	11.828	1618	1622	1626	rVB	53428	46784	1.48%	0.254%
19	13.033	1822	1827	1830	rBV	3001288	2623692	82.74%	14.231%
20	13.945	1967	1982	1997	rBV10	37878	180240	5.68%	0.978%
21	14.086	2002	2006	2009	rBV	422284	384880	12.14%	2.088%
22	15.580	2255	2260	2268	rBV	331117	429108	13.53%	2.328%

Sum of corrected areas: 18436163

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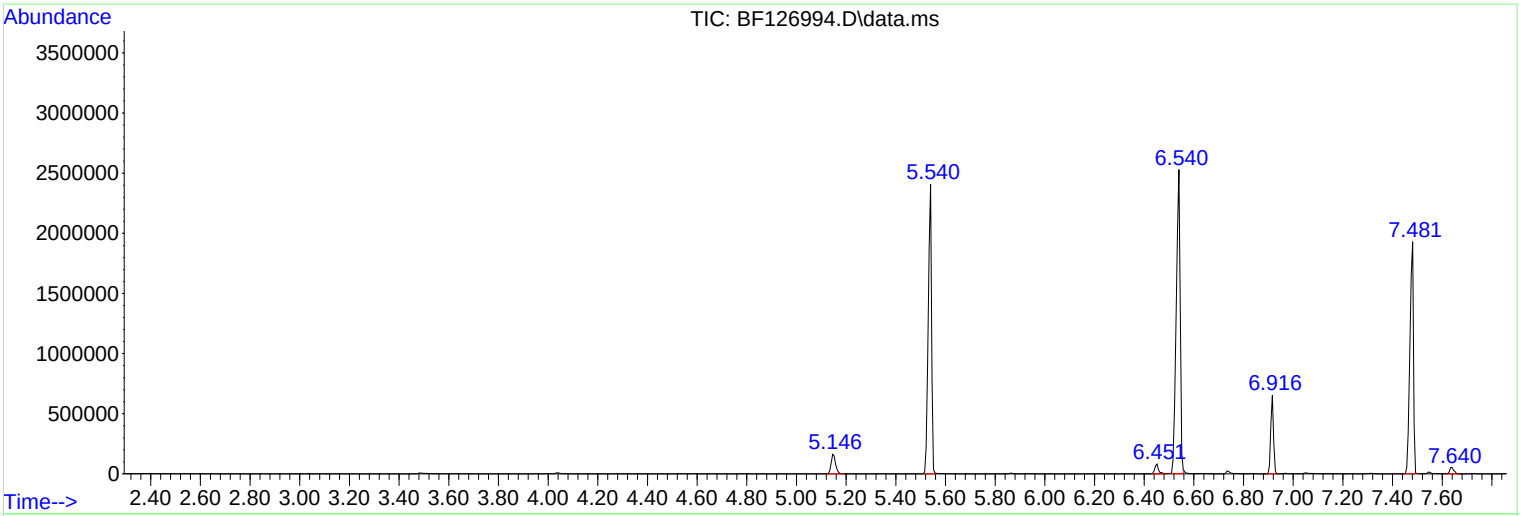
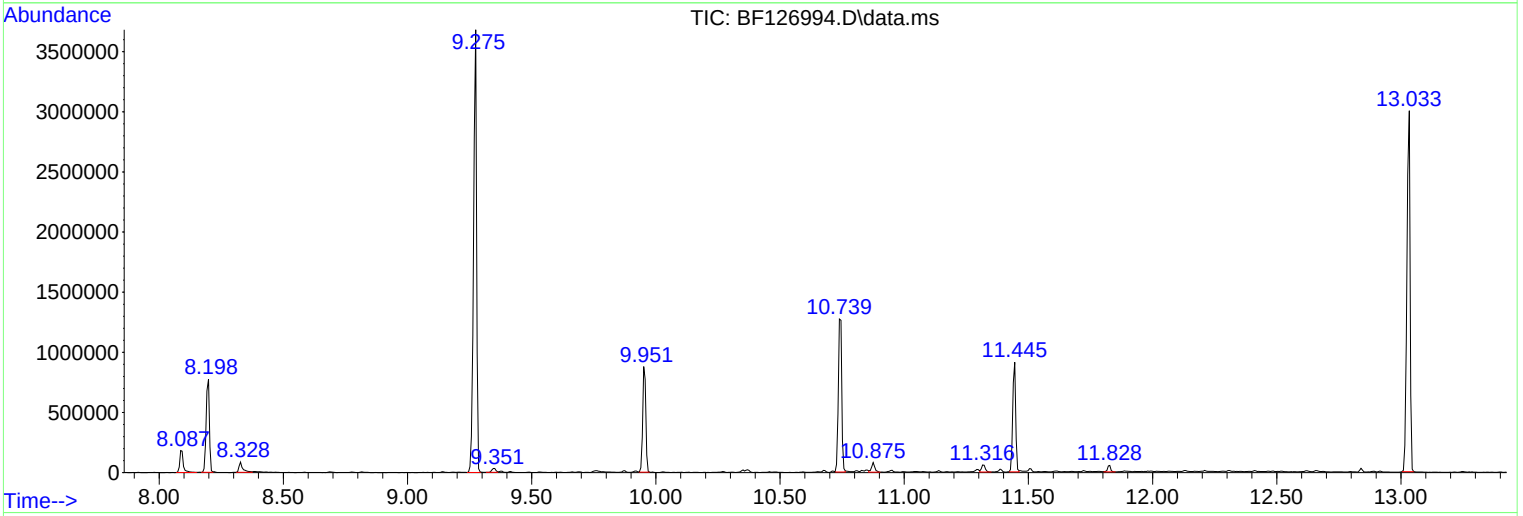
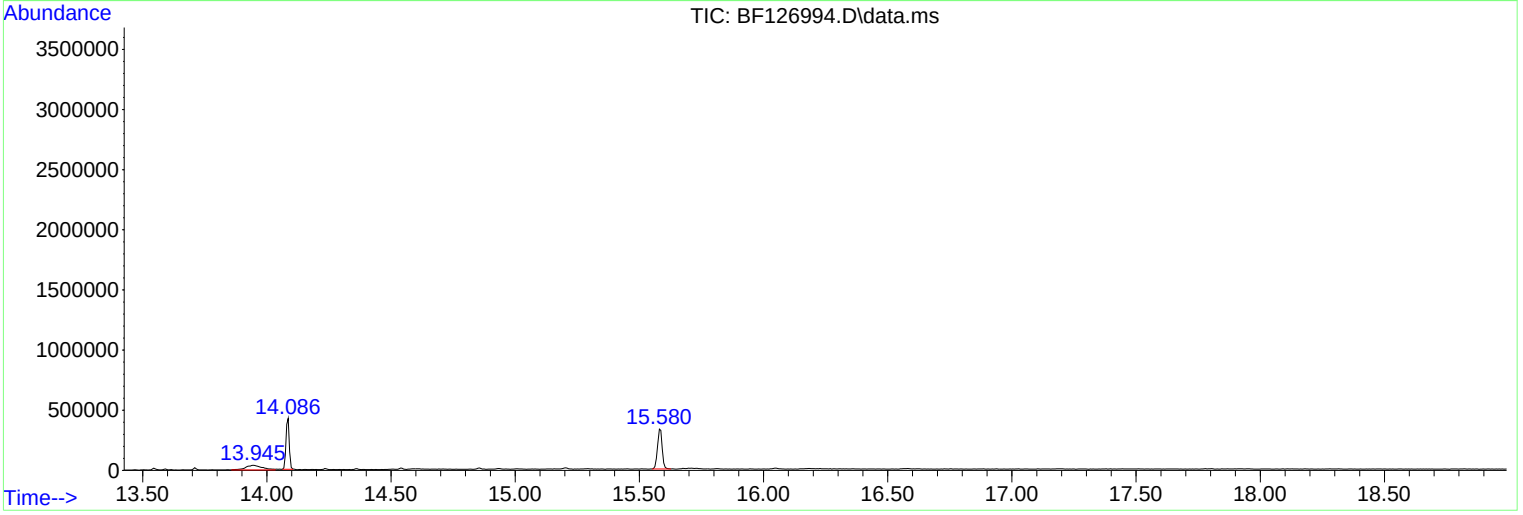
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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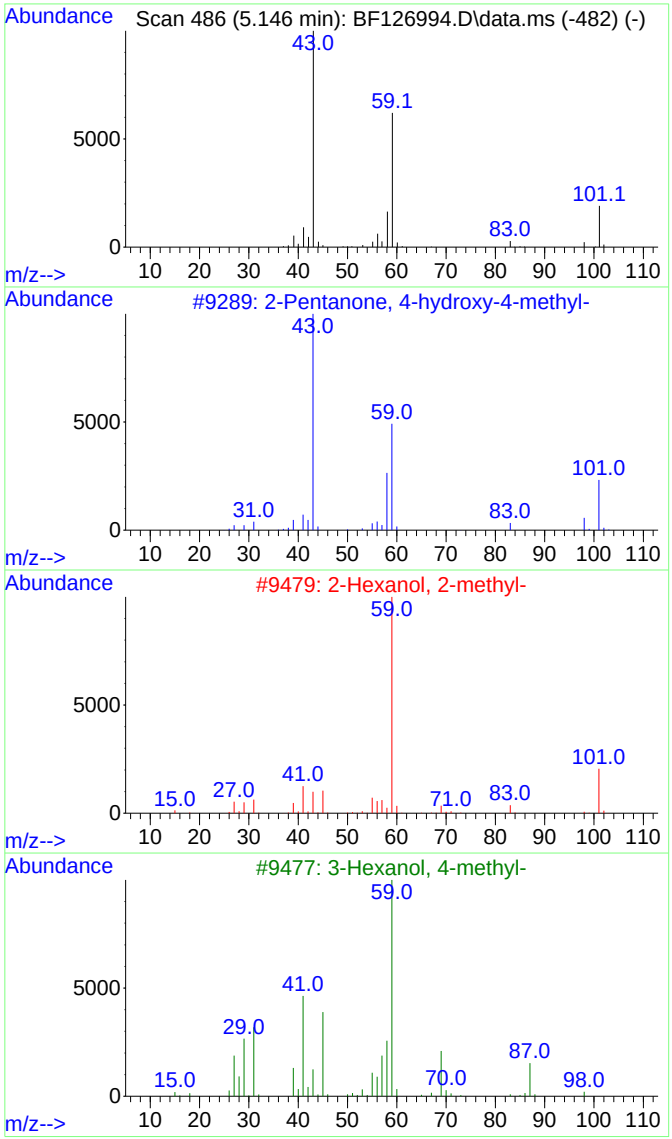
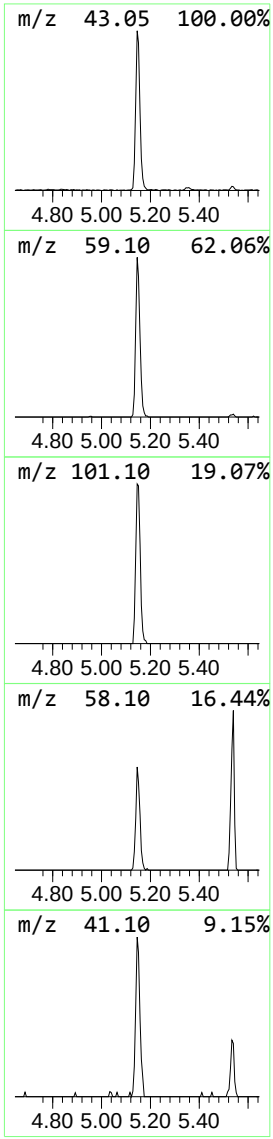
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.146	7.96 ng	200096	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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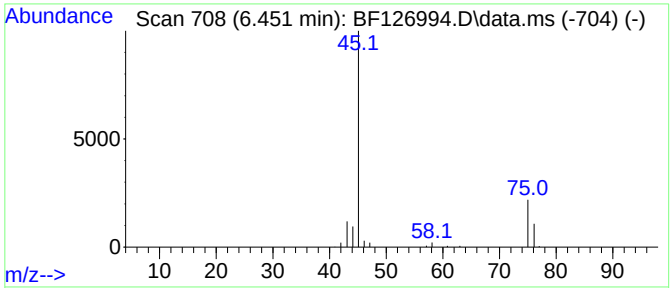
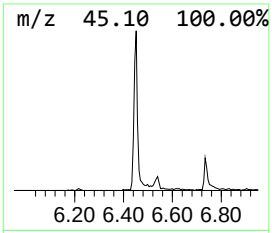
****

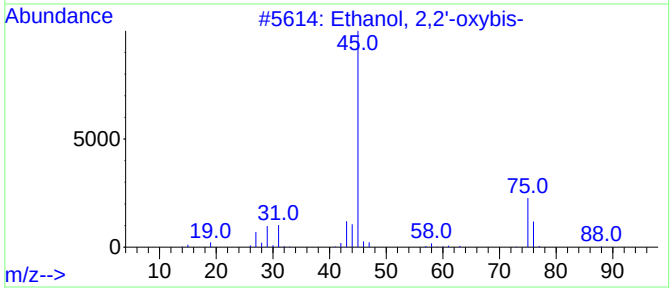
Peak Number 2 Ethanol, 2,2'-oxybis- Concentration Rank 4

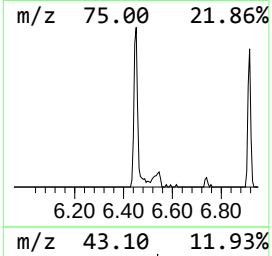
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.451	3.48 ng	87553	1,4-Dichlorobenzene-d4	6.916

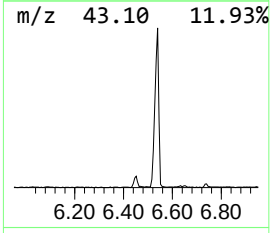
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	83
2	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9
3	2-Hydrazinoethanol	76	C2H8N2O	000109-84-2	9
4	Ethanol, 2-(2-hydroxyethoxy)-, 1...	151	C4H9NO5	020633-16-3	9
5	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9

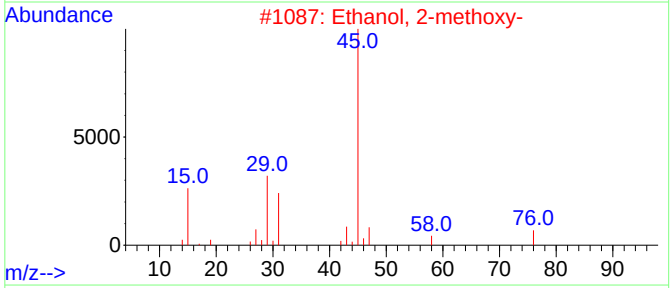


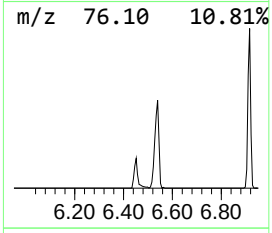


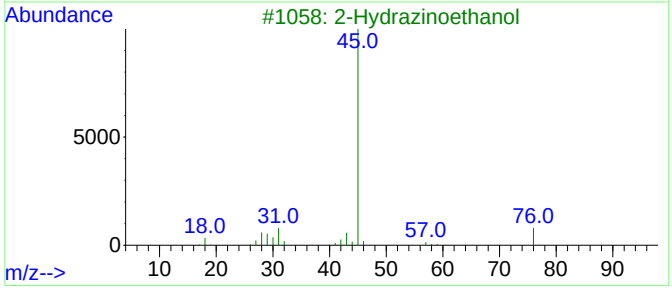


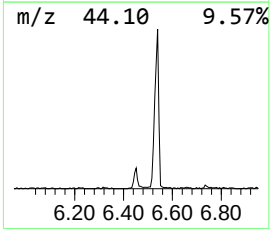












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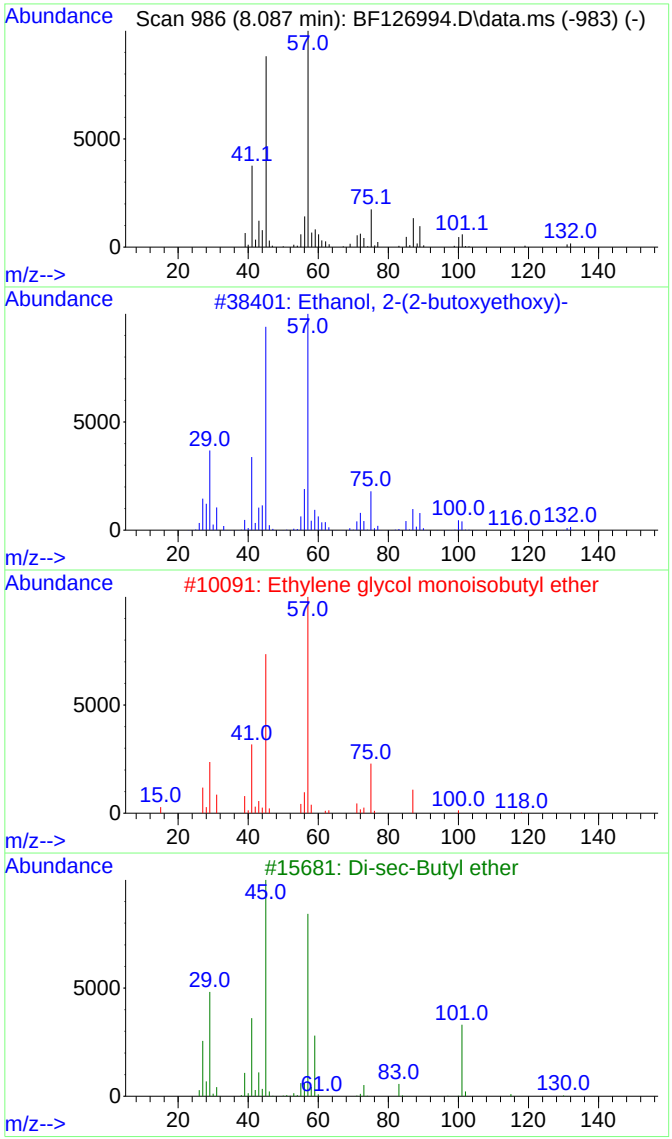
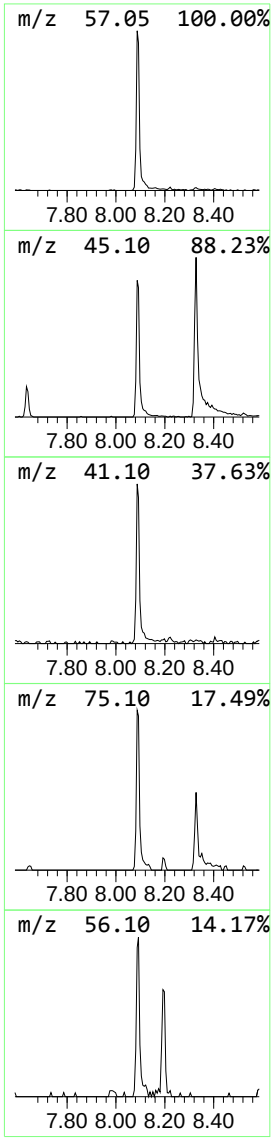
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.087	5.36 ng	183612	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	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5	Butyl lactate	146	C7H14O3	000138-22-7	47





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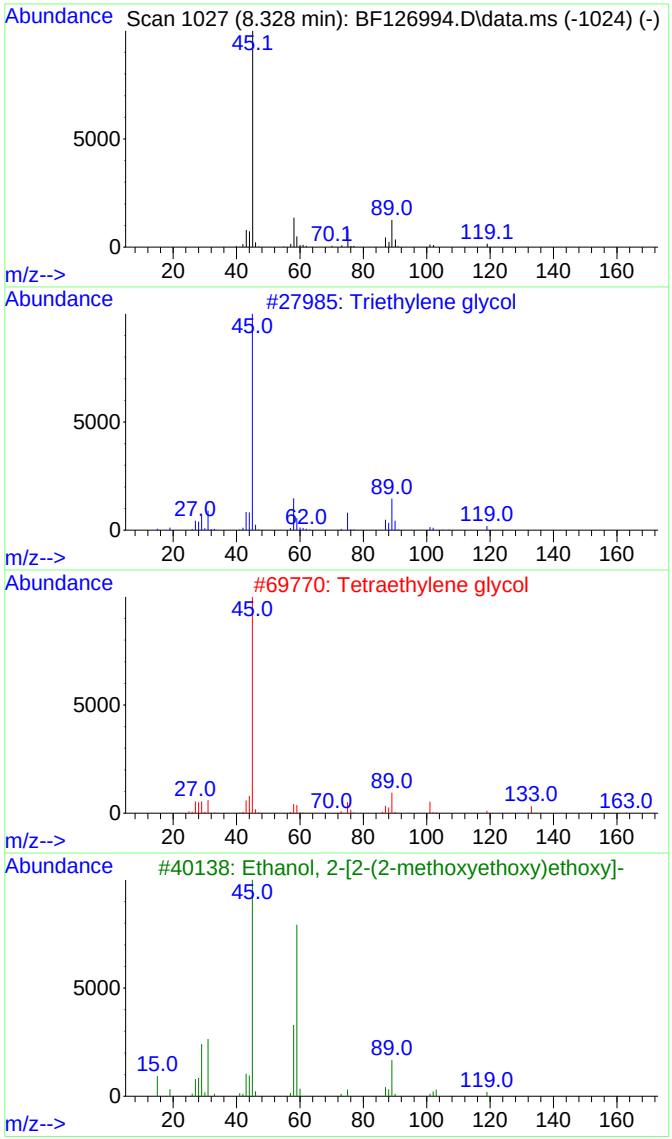
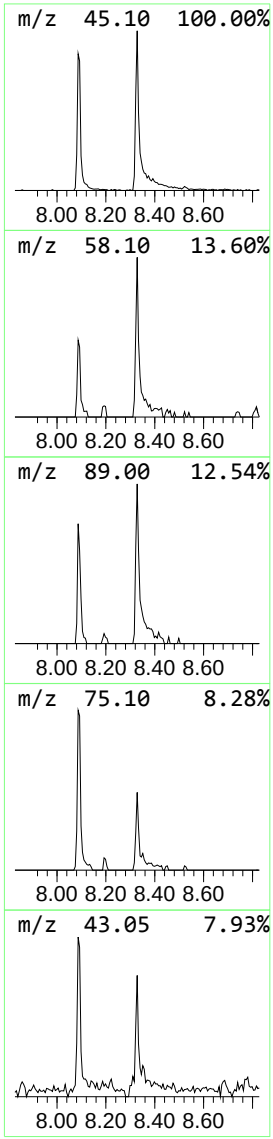
****

Peak Number 4 Triethylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.328	2.65 ng	90767	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethylene glycol	150	C6H14O4	000112-27-6	90
2	Tetraethylene glycol	194	C8H18O5	000112-60-7	78
3	Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	50
4	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	42
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	42





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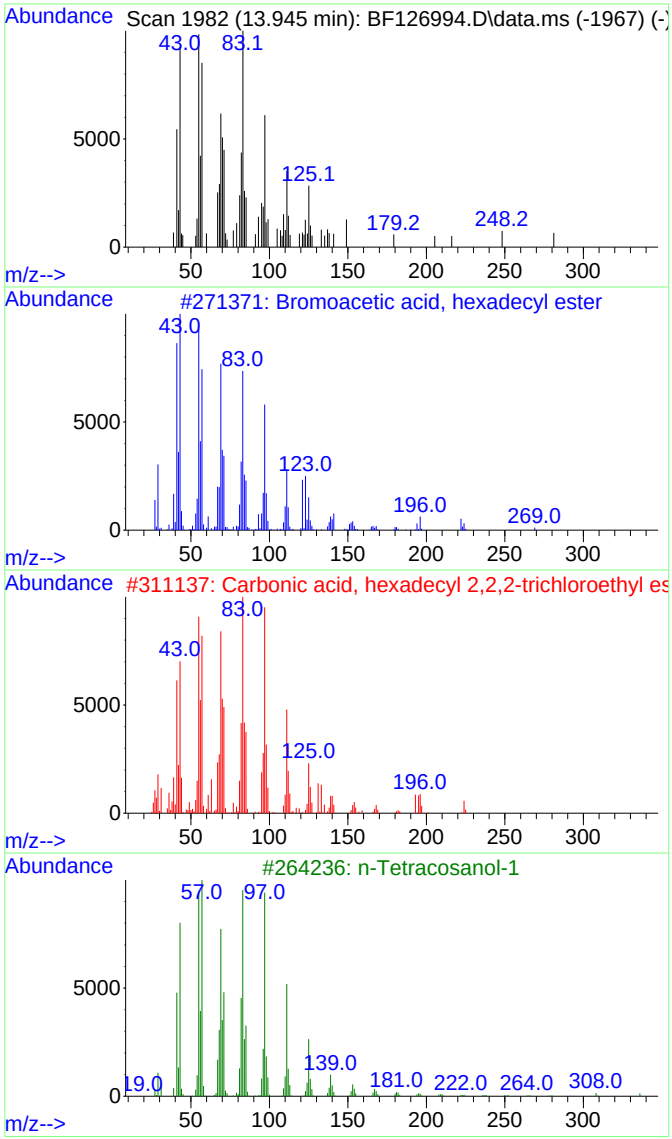
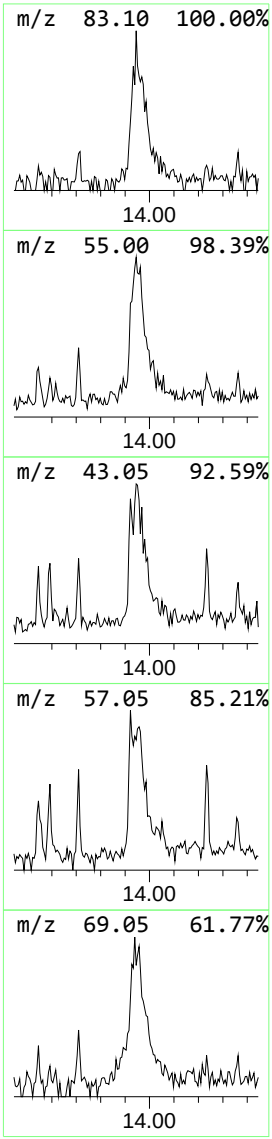
****
Peak Number 5 Bromoacetic acid, hexadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	9.37 ng	180240	Chrysene-d12	14.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
2	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	76
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
4	1-Tricosene	322	C23H46	018835-32-0	70
5	Behenic alcohol	326	C22H46O	000661-19-8	70





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.146	8.0	ng	200096	1	6.916	502716	20.0
Ethanol, 2,2'-o...	6.451	3.5	ng	87553	1	6.916	502716	20.0
Ethanol, 2-(2-b...	8.087	5.4	ng	183612	2	8.198	685167	20.0
Triethylene glycol	8.328	2.6	ng	90767	2	8.198	685167	20.0
Bromoacetic aci...	13.945	9.4	ng	180240	5	14.086	384880	20.0