LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103122\
Data File : BF130886.D
Acq On : 31 Oct 2022 18:47
Operator : CG\JU
Sample : N5355-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5518-2

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-BF102722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130886.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	12	16	21	rVB	47424	54871	2.04%	0.361%
2	2.257	22	29	35	rVB	1159652	1551506	57.65%	10.200%
3	2.381	45	50	57	rBV	29511	36872	1.37%	0.242%
4	5.163	519	523	531	rVB	137163	151578	5.63%	0.997%
5	5.557	585	590	593	rBV	1362604	1211537	45.02%	7.965%
6	6.551	755	759	763	rBV	911040	843687	31.35%	5.547%
7	6.939	821	825	829	rBV	591110	458777	17.05%	3.016%
8	7.504	916	921	924	rBV	1626110	1643162	61.06%	10.803%
9	8.122	1023	1026	1040	rBV	180672	305132	11.34%	2.006%
10	8.228	1040	1044	1047	rVB	679468	565671	21.02%	3.719%
11	9.304	1222	1227	1230	rBV	3032325	2691036	100.00%	17.692%
12	9.986	1339	1343	1347	rVB	705860	562435	20.90%	3.698%
13	10.780	1473	1478	1481	rBV	1677773	1450500	53.90%	9.536%
14	11.480	1593	1597	1600	rBV	633492	508697	18.90%	3.344%
15	13.074	1863	1868	1871	rBV	2281973	2176470	80.88%	14.309%
16	14.027	2025	2030	2038	rBV5	29664	77672	2.89%	0.511%
17	14.127	2043	2047	2050	rVV	492375	436785	16.23%	2.872%
18	14.221	2058	2063	2068	rBV	111486	120227	4.47%	0.790%
19	15.645	2300	2305	2310	rBV	287549	363865	13.52%	2.392%

Sum of corrected areas: 15210480

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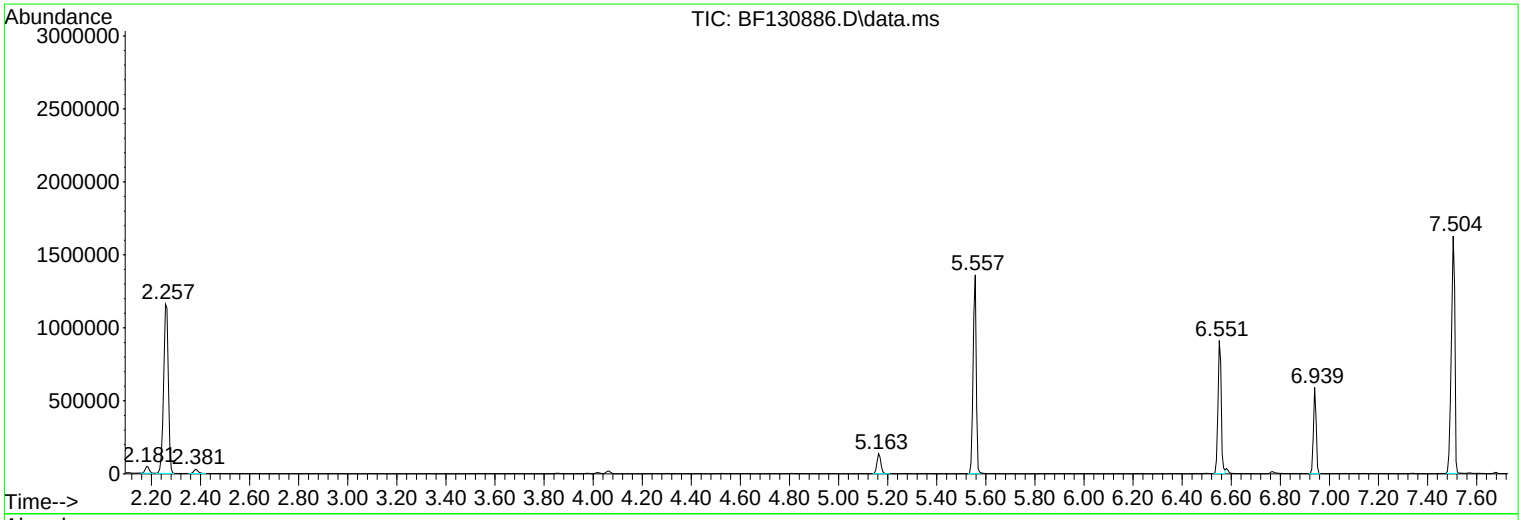
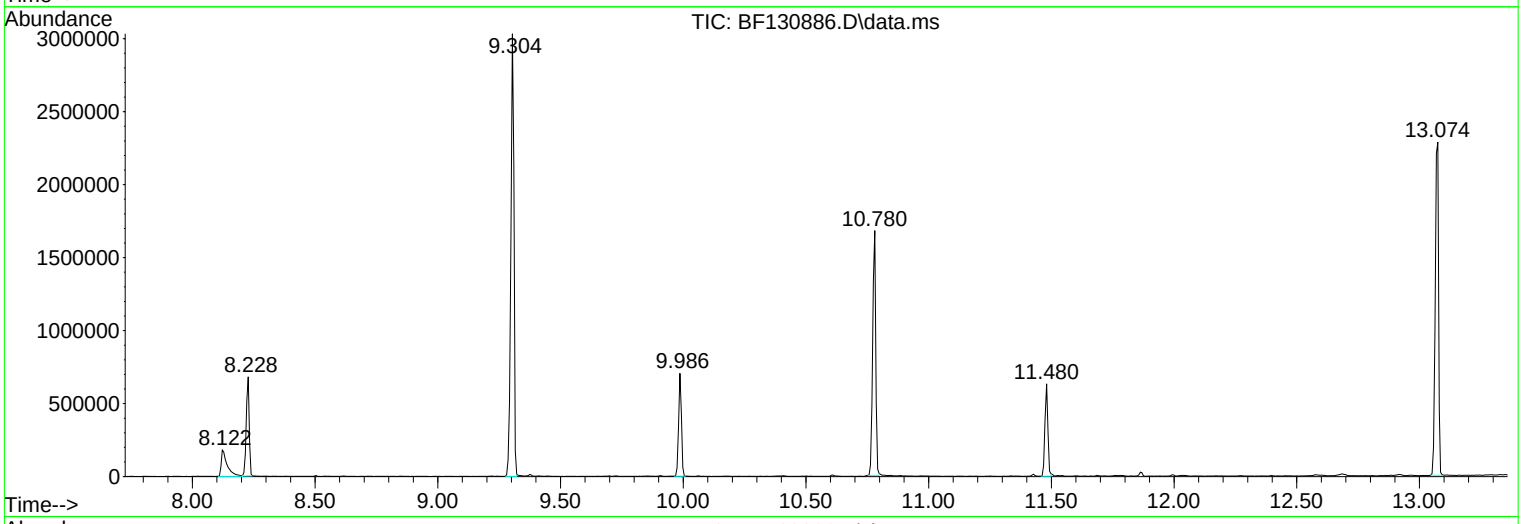
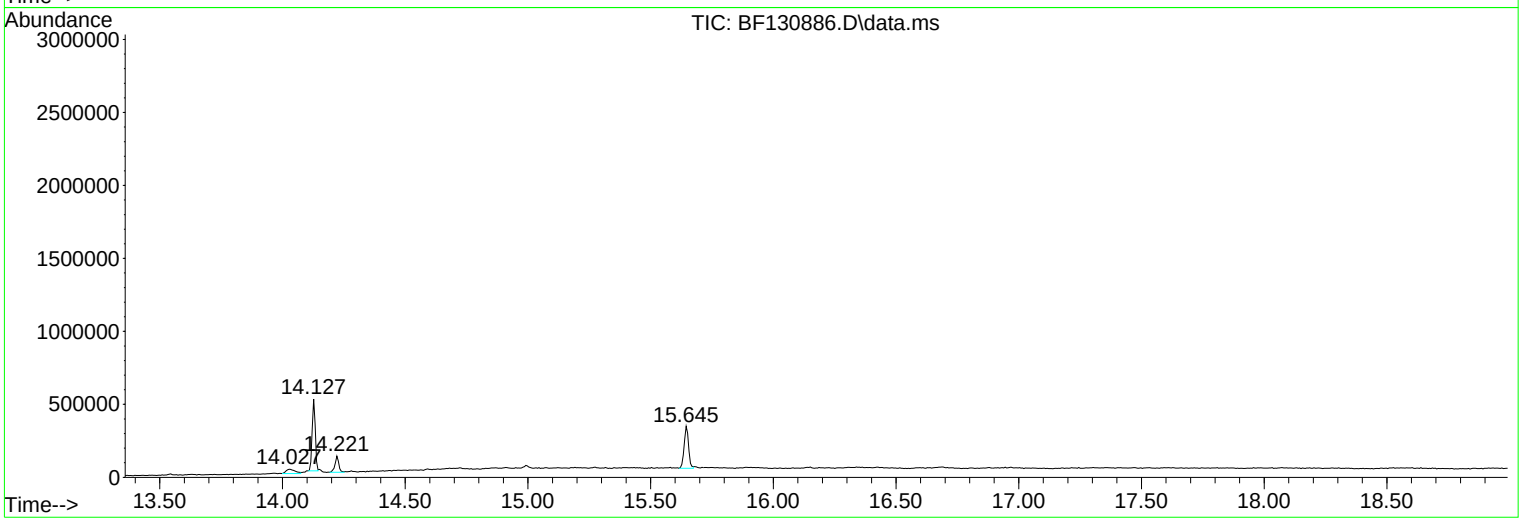
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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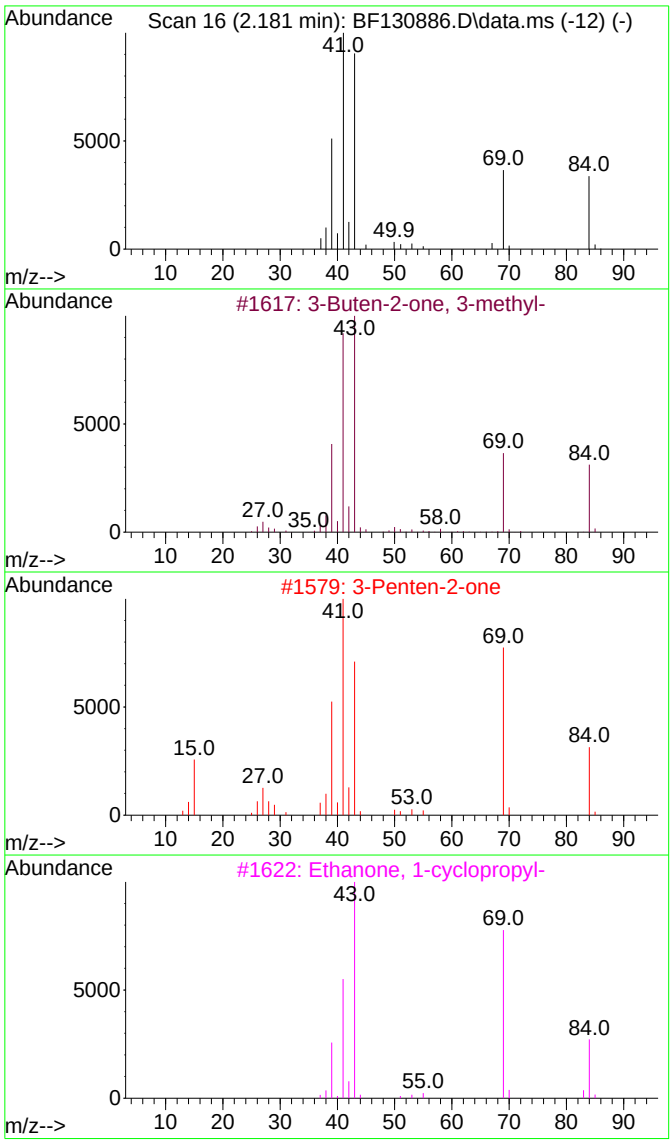
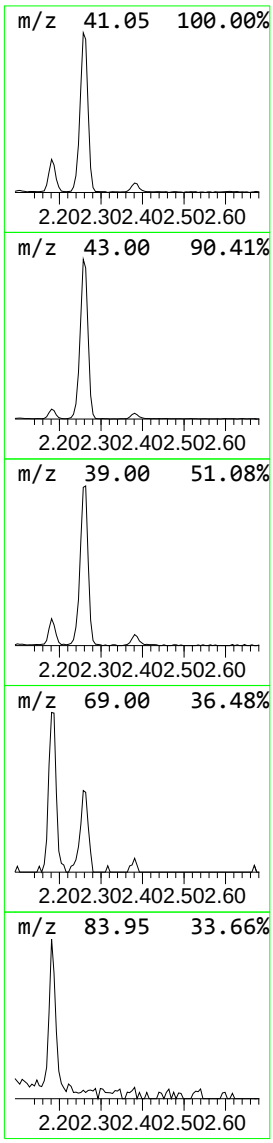
****

Peak Number 1 3-Buten-2-one, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	2.39 ng	54871	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2	3-Penten-2-one	84	C5H8O	000625-33-2	83
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	83
4	Cyclopropane, 1,1,2-trimethyl-	84	C6H12	004127-45-1	35
5	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

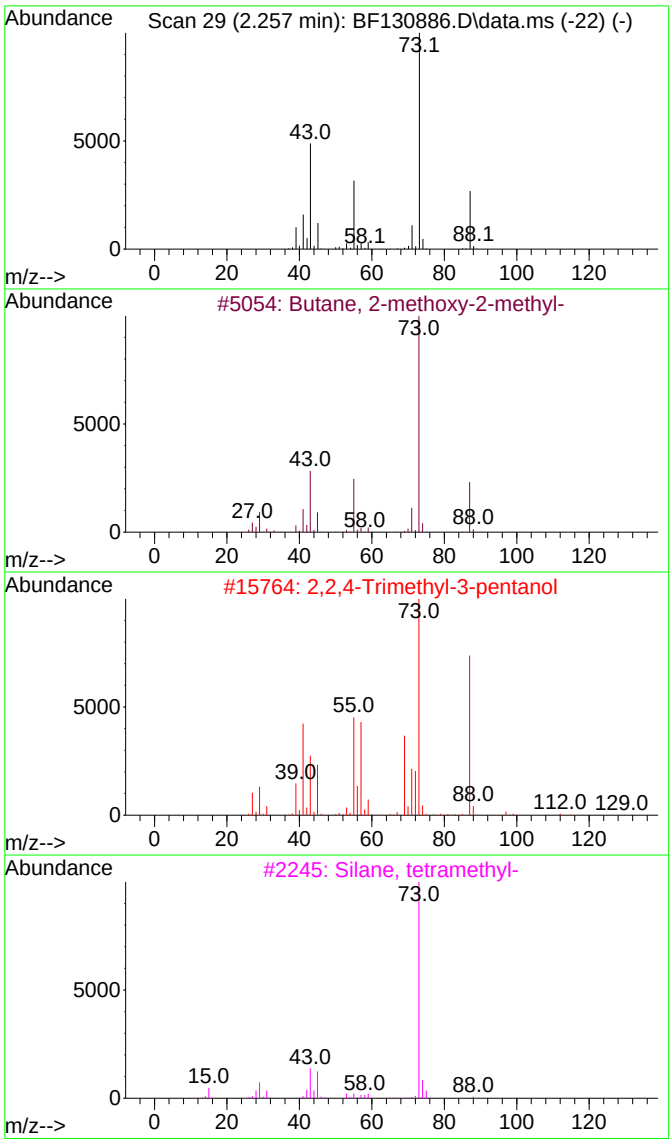
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

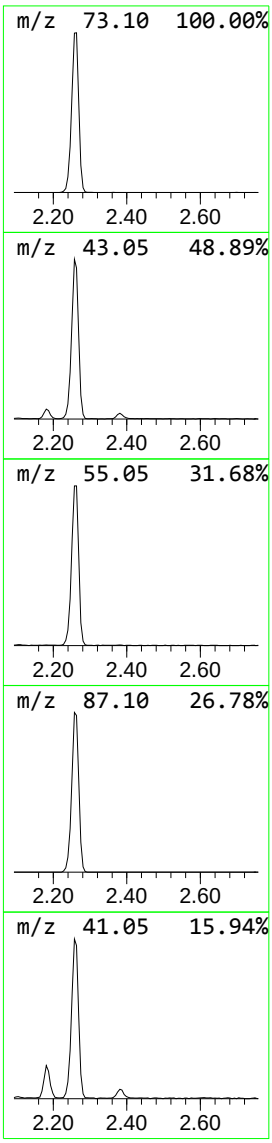
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	67.64 ng	1551510	1,4-Dichlorobenzene-d4	6.939

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	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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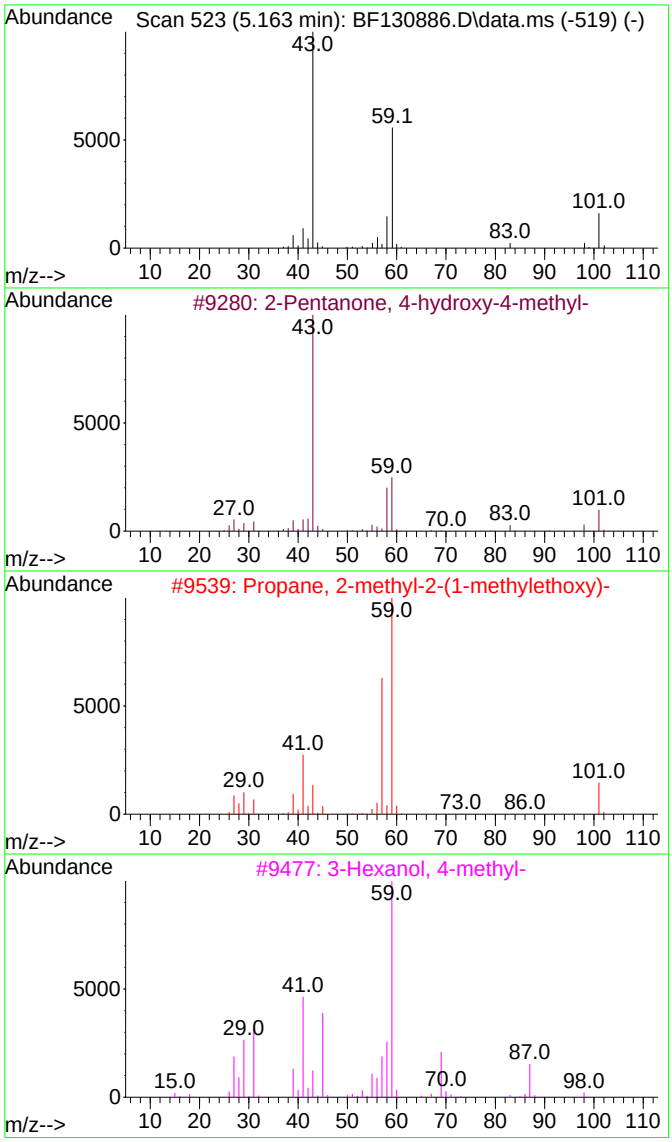
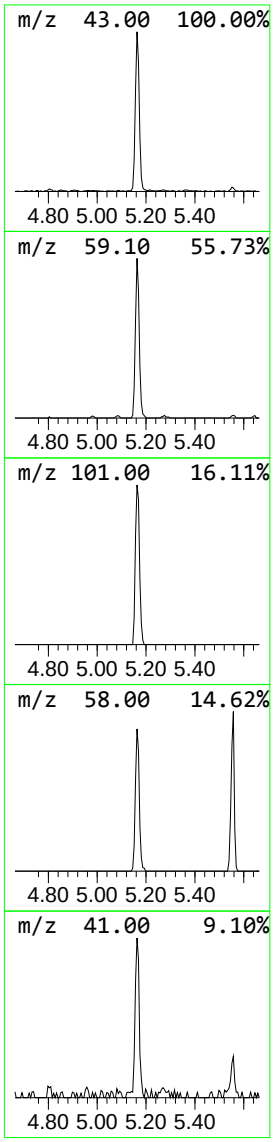
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	6.61 ng	151578	1,4-Dichlorobenzene-d4	6.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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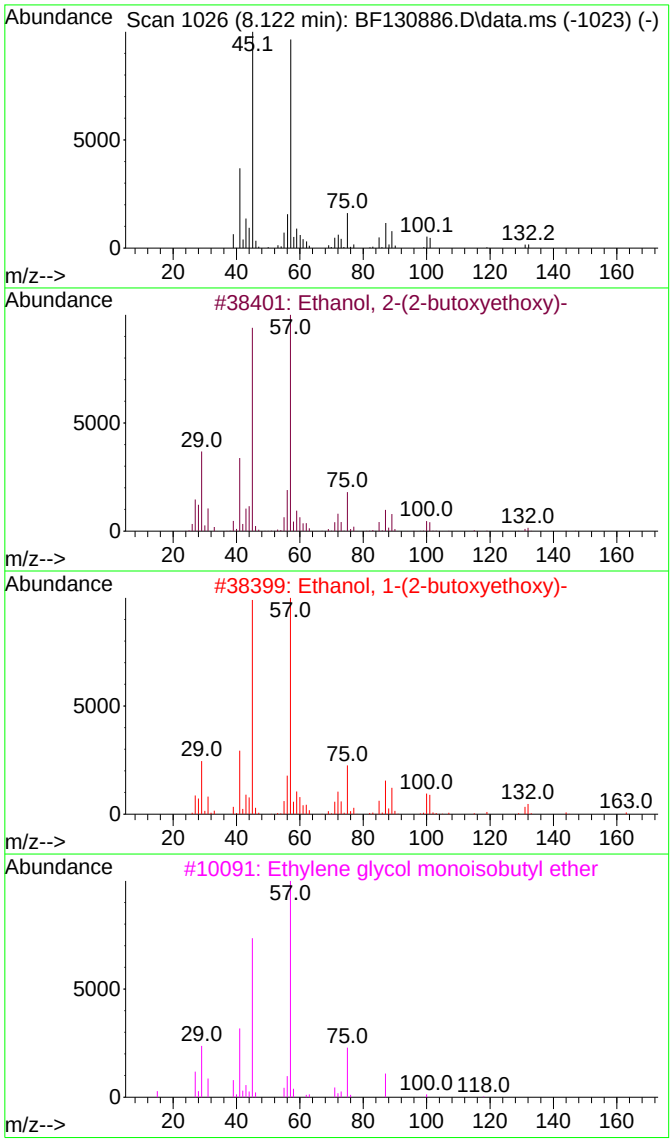
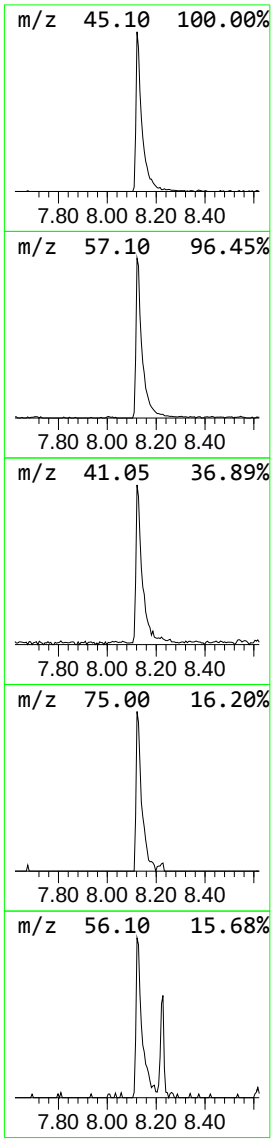
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.122	10.79 ng	305132	Naphthalene-d8	8.228

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	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
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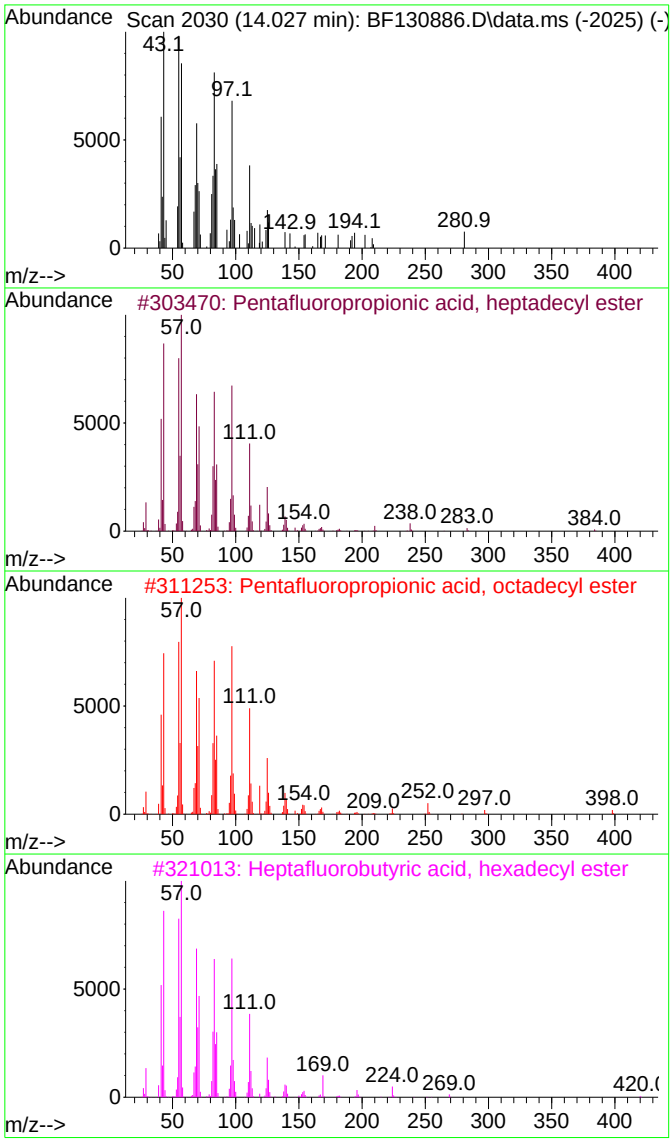
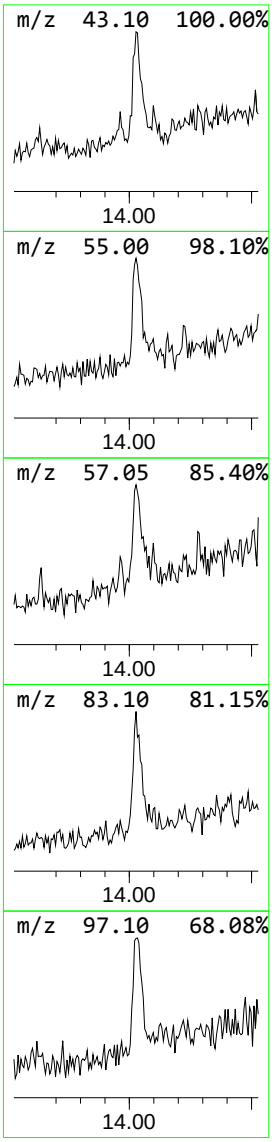
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.027	3.56 ng	77672	Chrysene-d12	14.127

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	87
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	87
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83





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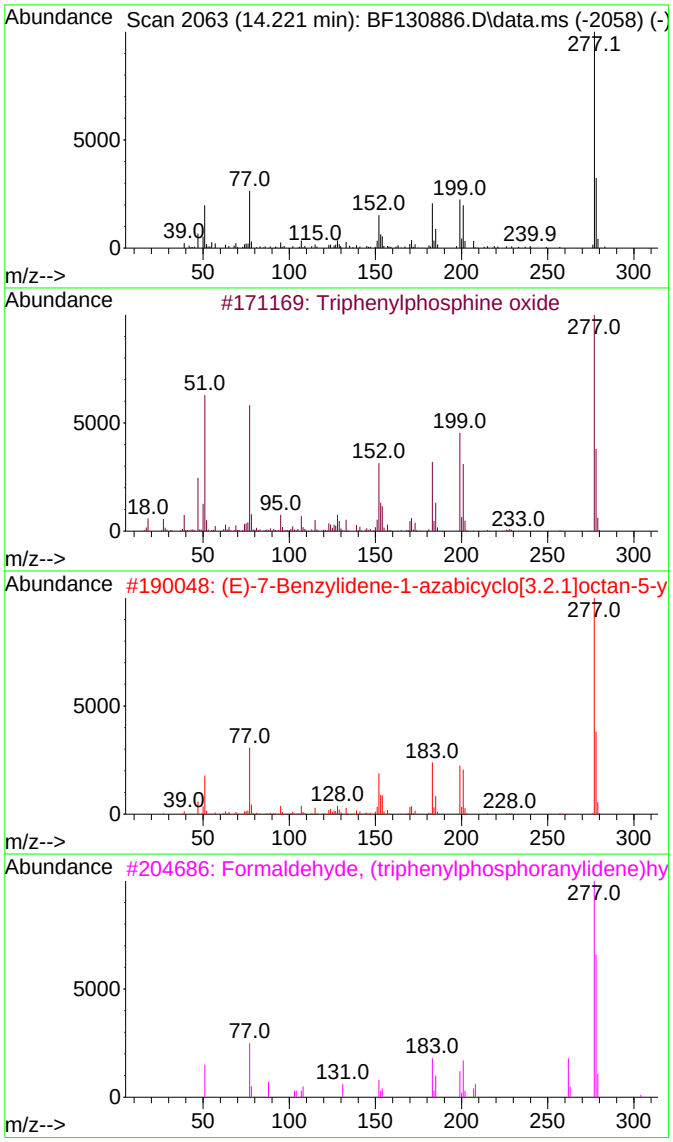
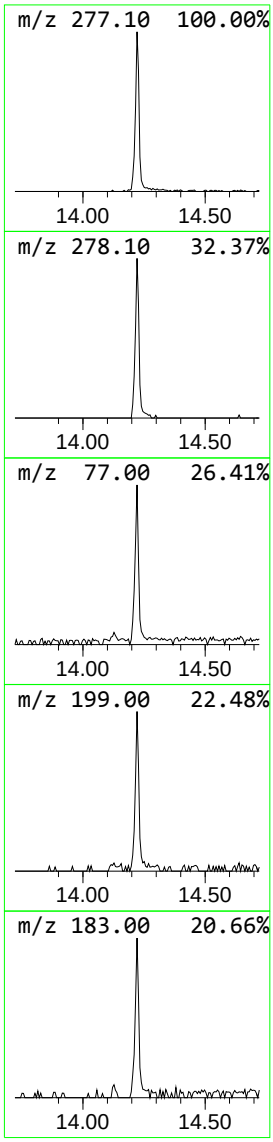
Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.221	5.51 ng	120227	Chrysene-d12	14.127

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Buten-2-one, ...	2.181	2.4	ng	54871	1	6.939	458777	20.0
Butane, 2-metho...	2.257	67.6	ng	1551510	1	6.939	458777	20.0
2-Pentanone, 4-...	5.163	6.6	ng	151578	1	6.939	458777	20.0
Ethanol, 2-(2-b...	8.122	10.8	ng	305132	2	8.228	565671	20.0
Pentafluoroprop...	14.027	3.6	ng	77672	5	14.127	436785	20.0
Triphenylphosph...	14.221	5.5	ng	120227	5	14.127	436785	20.0