LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
Data File : BF131427.D
Acq On : 28 Nov 2022 13:34
Operator : CG\JU
Sample : N5766-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CR-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-BF112122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131427.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	22	36	44	rVB	512817	719810	28.23%	4.150%
2	2.410	50	55	61	rVB	22249	28536	1.12%	0.165%
3	5.181	521	526	535	rVB	375456	493686	19.36%	2.846%
4	5.569	587	592	595	rBV	2163746	2122160	83.22%	12.235%
5	6.569	756	762	765	rBV	2033680	2133670	83.67%	12.301%
6	6.951	823	827	830	rVB	630209	489246	19.18%	2.821%
7	7.516	917	923	926	rBV	1440392	1381171	54.16%	7.963%
8	8.239	1041	1046	1049	rBV	757811	637909	25.01%	3.678%
9	8.857	1147	1151	1154	rBV	185943	144928	5.68%	0.836%
10	9.322	1224	1230	1233	rBV	2849971	2550156	100.00%	14.702%
11	10.004	1341	1346	1349	rBV	922111	748677	29.36%	4.316%
12	10.798	1476	1481	1484	rBV	1903270	1642040	64.39%	9.467%
13	11.498	1596	1600	1604	rBV	822995	750341	29.42%	4.326%
14	13.098	1867	1872	1875	rBV	2774064	2432923	95.40%	14.027%
15	13.998	2021	2025	2039	rBV	70119	141262	5.54%	0.814%
16	14.157	2048	2052	2055	rBV	574051	482682	18.93%	2.783%
17	14.251	2064	2068	2075	rVB	44191	48340	1.90%	0.279%
18	15.692	2308	2313	2317	rBV2	331504	397566	15.59%	2.292%

Sum of corrected areas: 17345103

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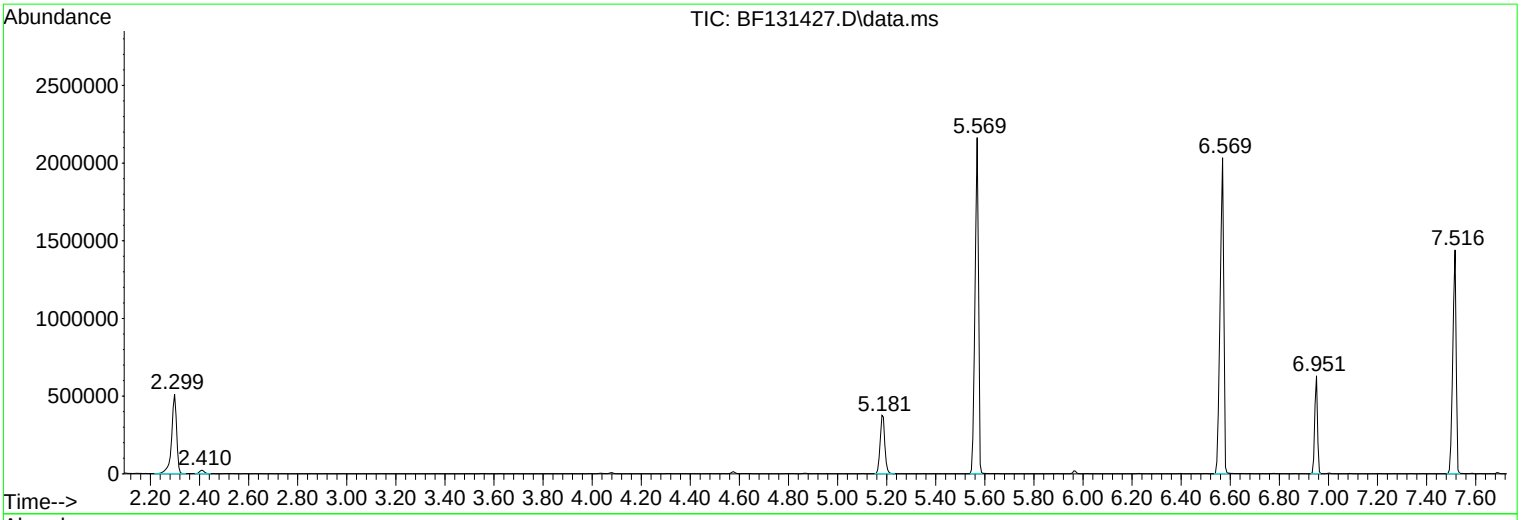
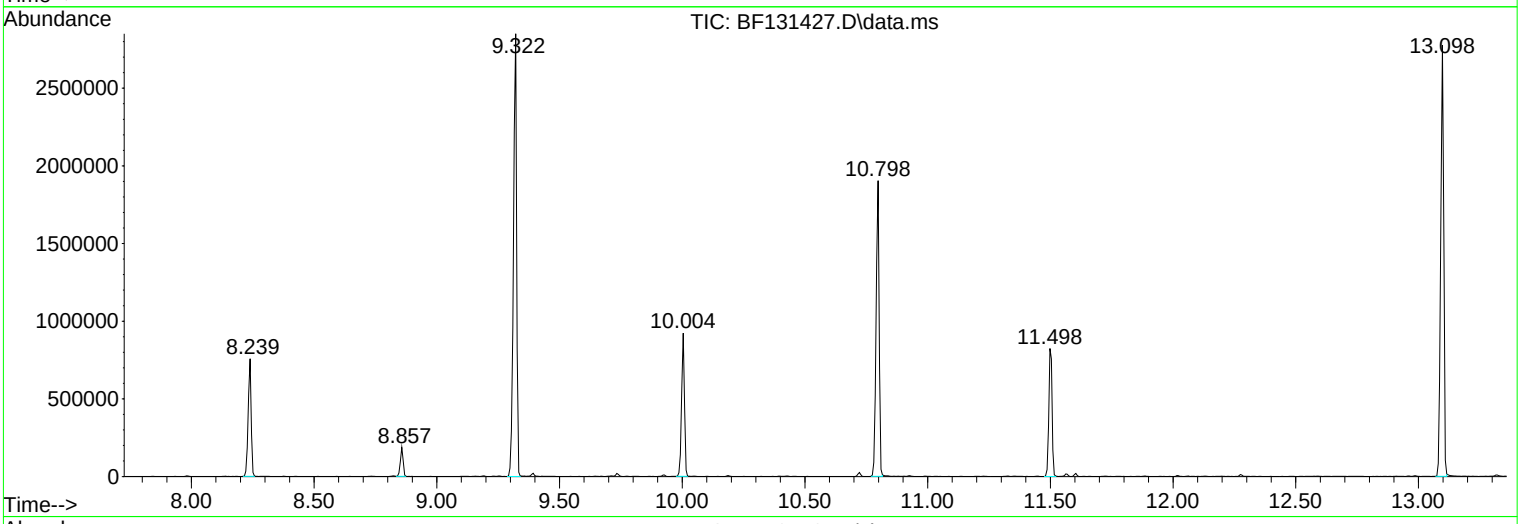
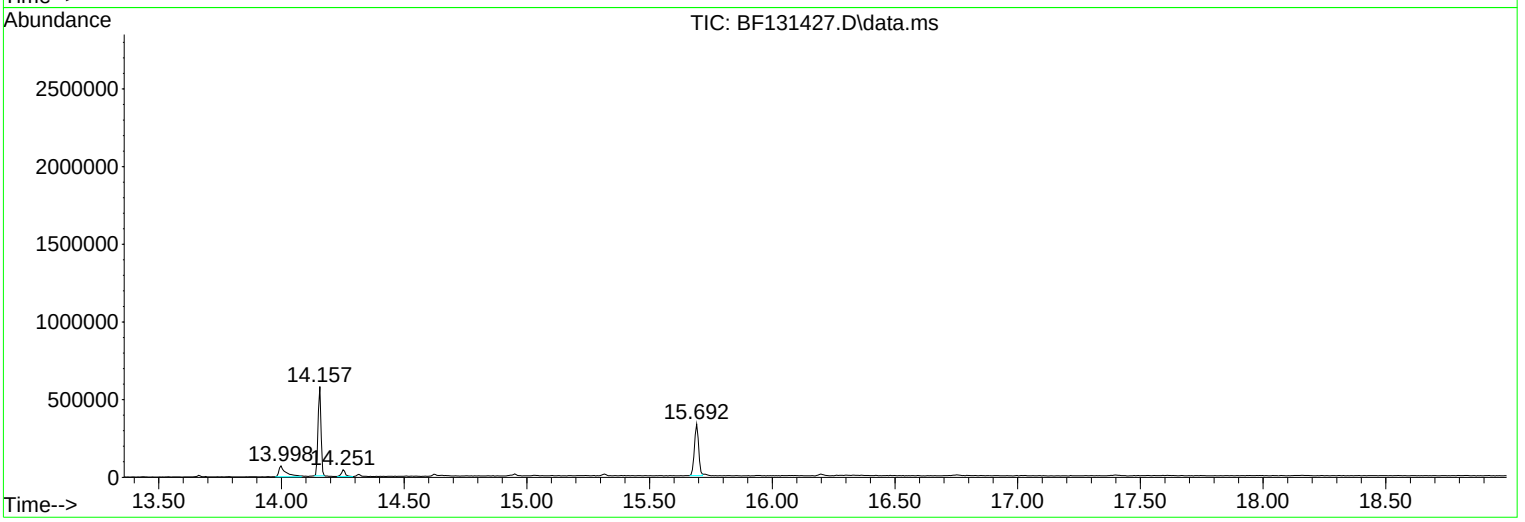
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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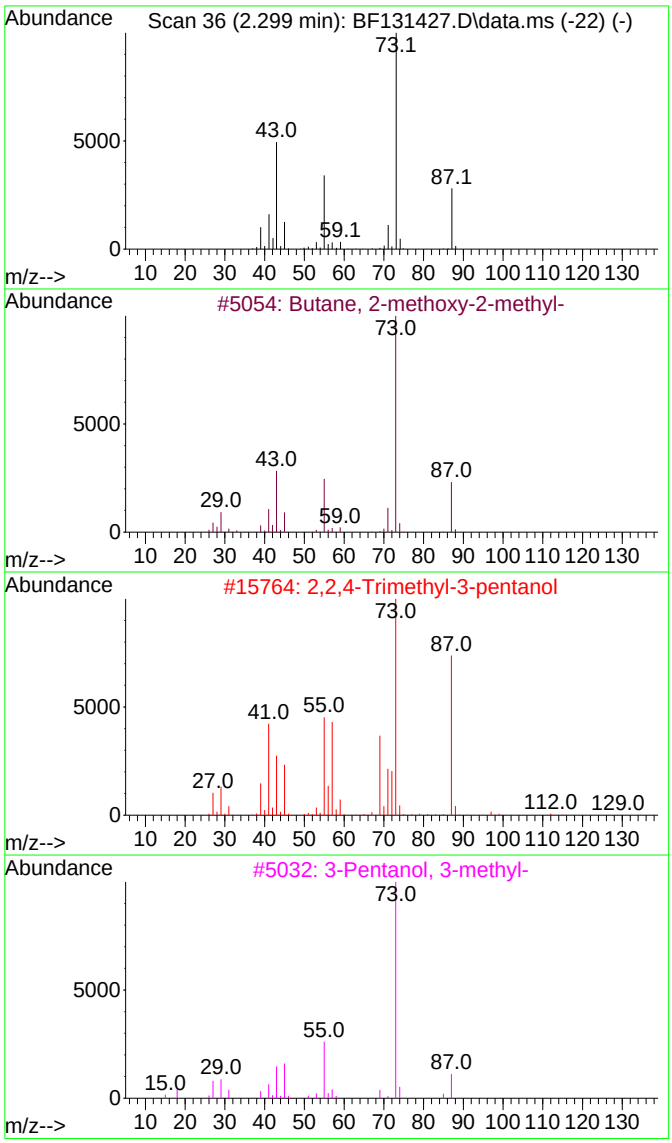
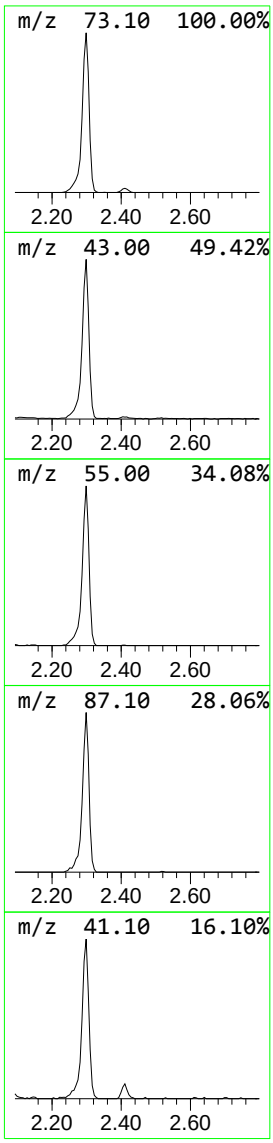
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	29.43 ng	719810	1,4-Dichlorobenzene-d4	6.951

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	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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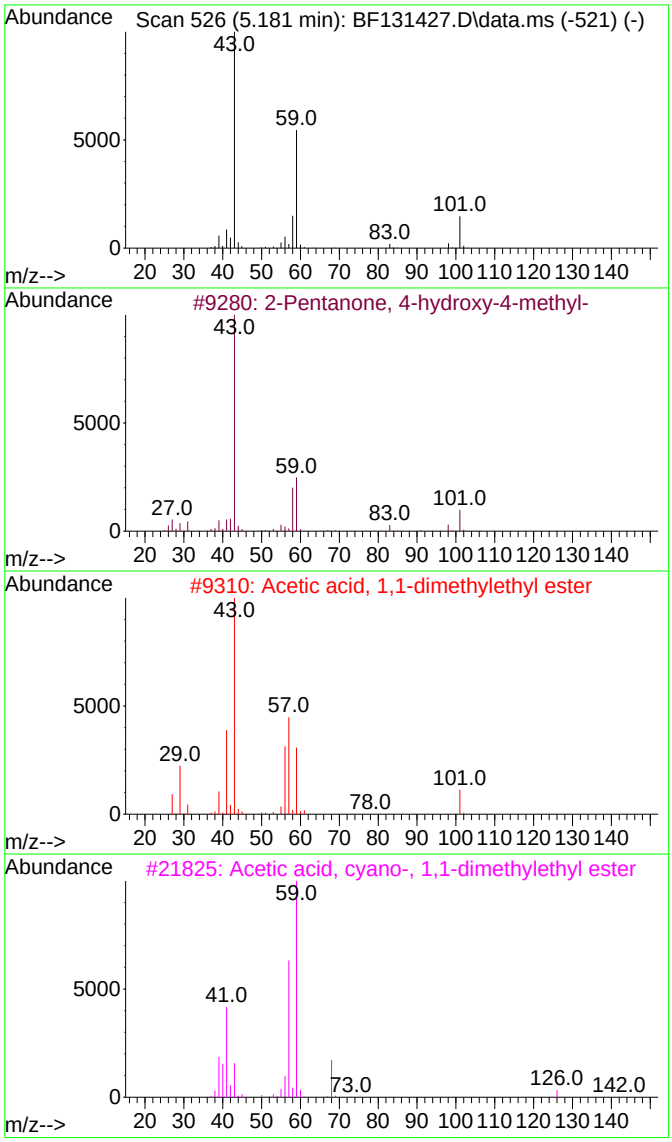
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

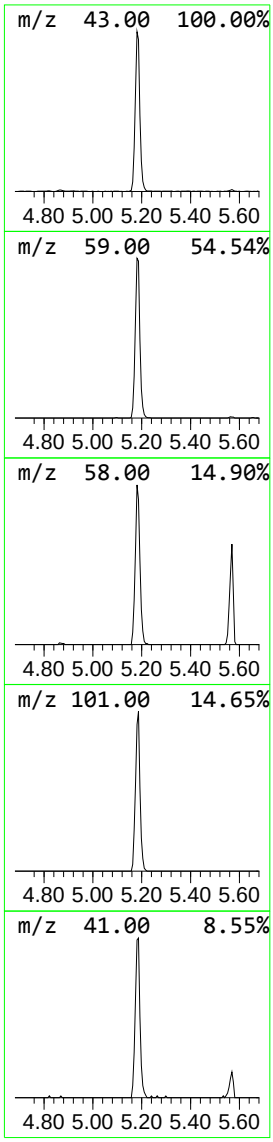
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	20.18 ng	493686	1,4-Dichlorobenzene-d4	6.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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BNA_F
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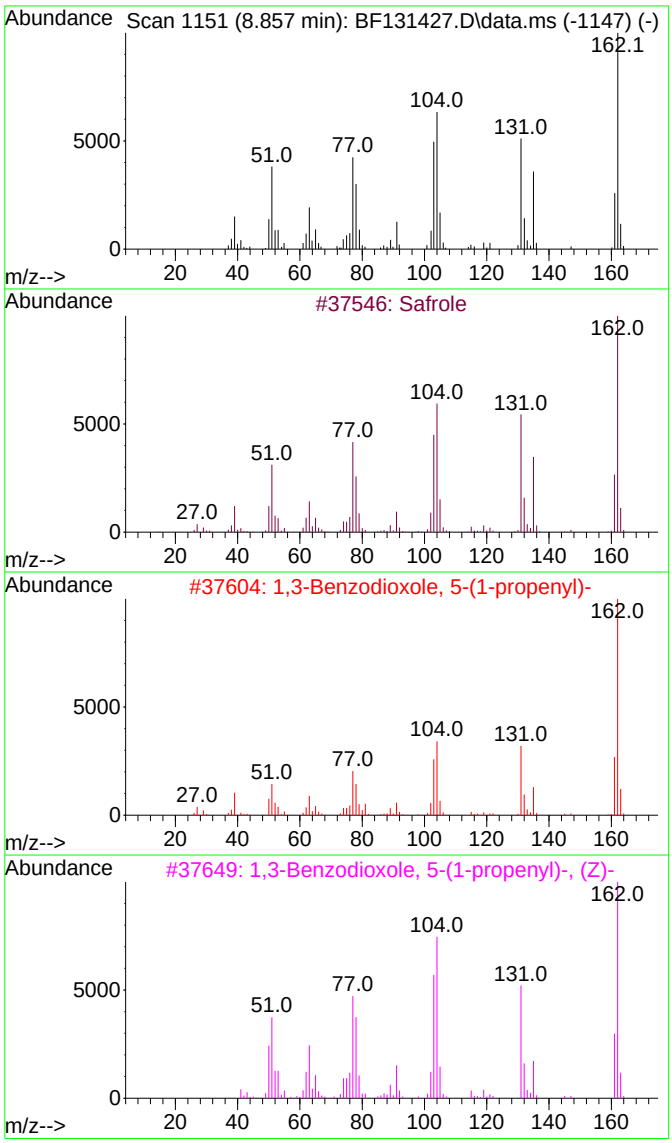
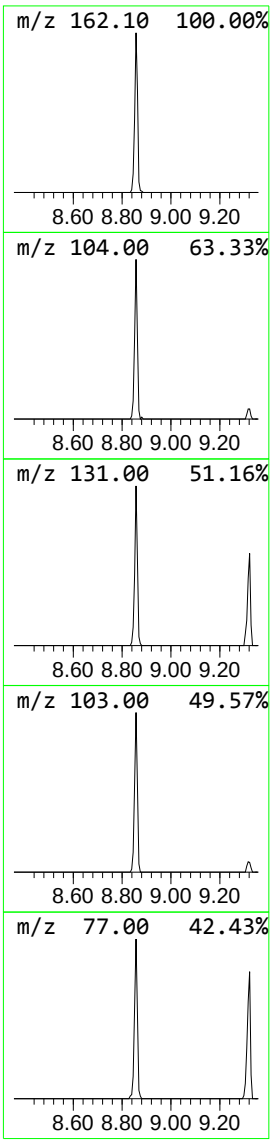
****

Peak Number 3 Safrole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.857	4.54 ng	144928	Naphthalene-d8	8.239

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safrole	162	C10H10O2	000094-59-7	98
2	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	97
4	Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	95
5	Sydnone, 3-phenyl-	162	C8H6N2O2	000120-06-9	52





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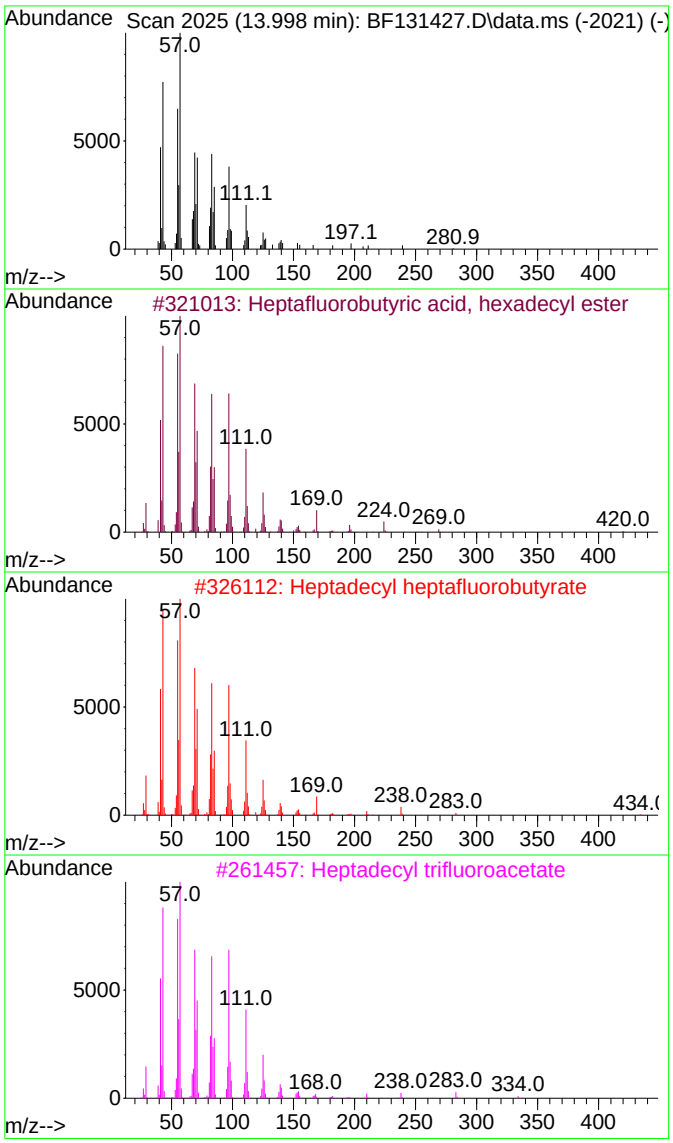
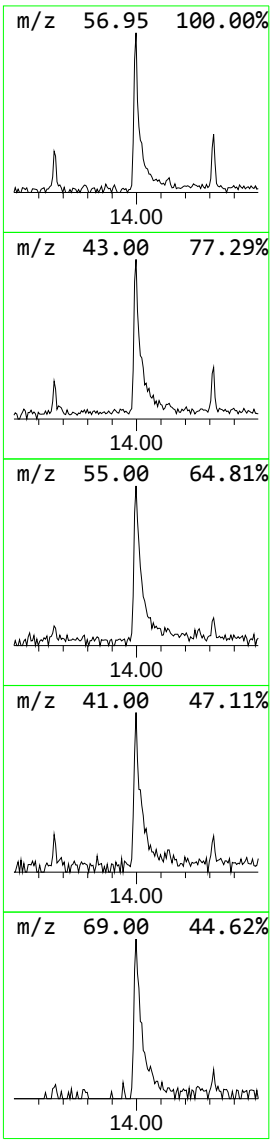
****
Peak Number 4 Heptafluorobutyric acid, he... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	5.85 ng	141262	Chrysene-d12	14.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91





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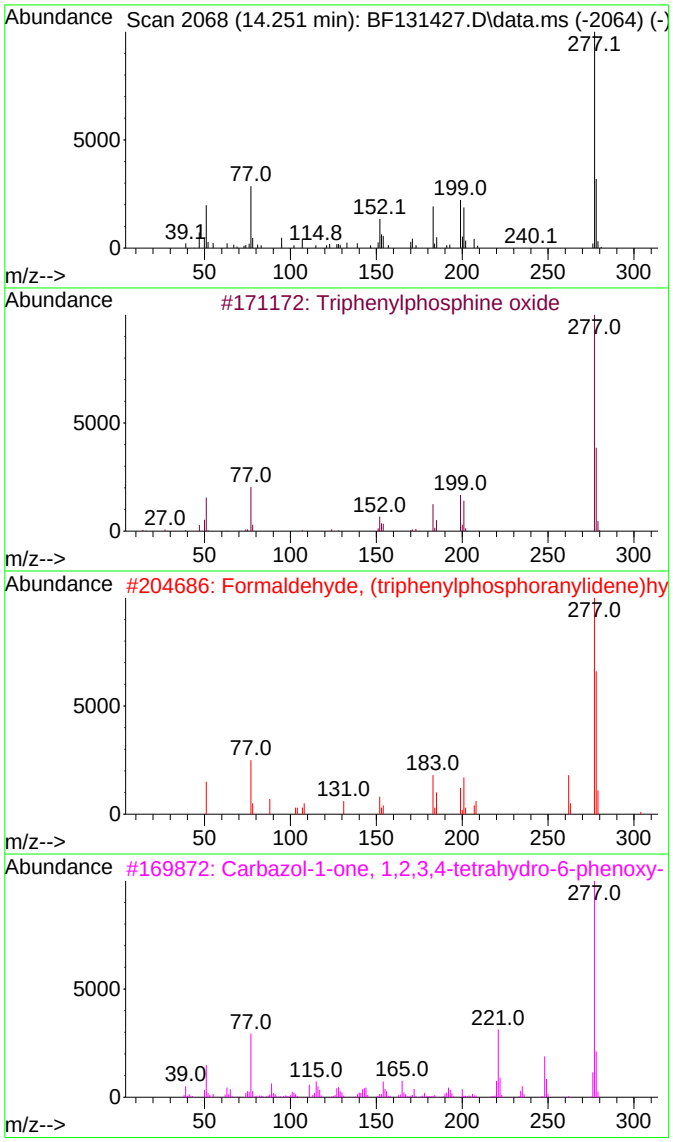
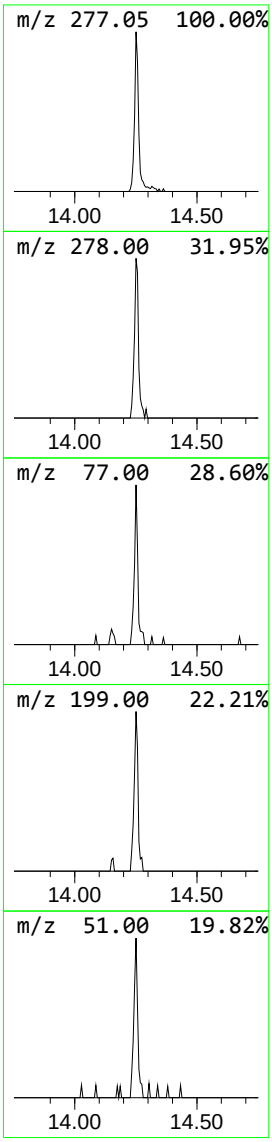
****
Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	2.00 ng	48340	Chrysene-d12	14.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	39
3	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38
4	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	38
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	32





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...	2.299	29.4	ng	719810	1	6.951	489246	20.0
2-Pentanone, 4-...	5.181	20.2	ng	493686	1	6.951	489246	20.0
Safrole	8.857	4.5	ng	144928	2	8.239	637909	20.0
Heptafluorobuty...	13.998	5.8	ng	141262	5	14.157	482682	20.0
Triphenylphosph...	14.251	2.0	ng	48340	5	14.157	482682	20.0