LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031423\
Data File : BF132780.D
Acq On : 14 Mar 2023 16:12
Operator : CG\JU
Sample : 01891-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C0AA7

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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132780.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.593	337	341	348	rBV	119919	136109	2.26%	0.425%
2	5.192	439	443	451	rBV	882041	917122	15.25%	2.861%
3	5.592	507	511	522	rBV	2170843	2019757	33.59%	6.301%
4	5.981	573	577	583	rBV	171948	162741	2.71%	0.508%
5	6.592	677	681	694	rBV	1247902	1204573	20.03%	3.758%
6	6.963	741	744	748	rBV	1434254	1149903	19.12%	3.587%
7	7.534	836	841	844	rBV	3373603	3334919	55.46%	10.404%
8	8.245	959	962	966	rBV	1764046	1484776	24.69%	4.632%
9	9.322	1141	1145	1148	rBV	5879660	5609571	93.29%	17.500%
10	10.004	1258	1261	1265	rBV	1854407	1729197	28.76%	5.395%
11	10.722	1379	1383	1386	rBV	301297	236771	3.94%	0.739%
12	10.804	1392	1397	1400	rBV	3971951	3721182	61.89%	11.609%
13	11.498	1512	1515	1519	rBV	2013479	1820506	30.28%	5.679%
14	13.092	1781	1786	1789	rBV	6245236	6012854	100.00%	18.758%
15	13.968	1931	1935	1945	rBV	82158	139325	2.32%	0.435%
16	14.110	1955	1959	1963	rBV	72452	65309	1.09%	0.204%
17	14.157	1963	1967	1976	rVB	1174253	1084004	18.03%	3.382%
18	14.998	2106	2110	2117	rVB2	72702	88799	1.48%	0.277%
19	15.686	2222	2227	2237	rVB2	871043	1137115	18.91%	3.547%

Sum of corrected areas: 32054533

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ClientSampleId :
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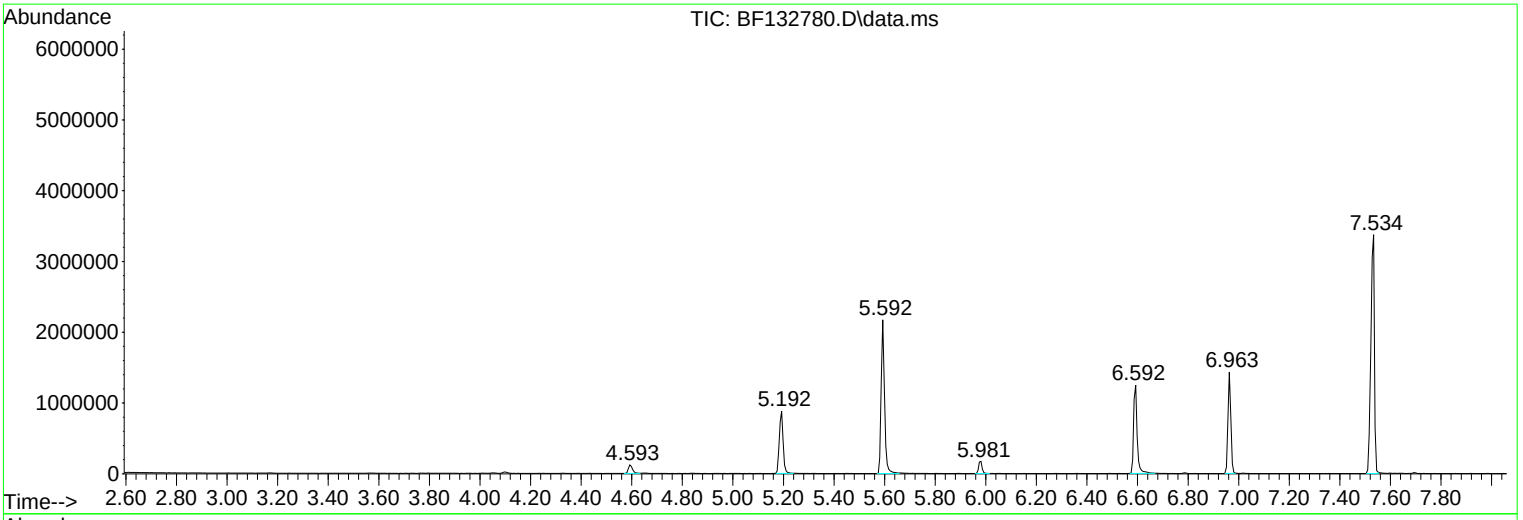
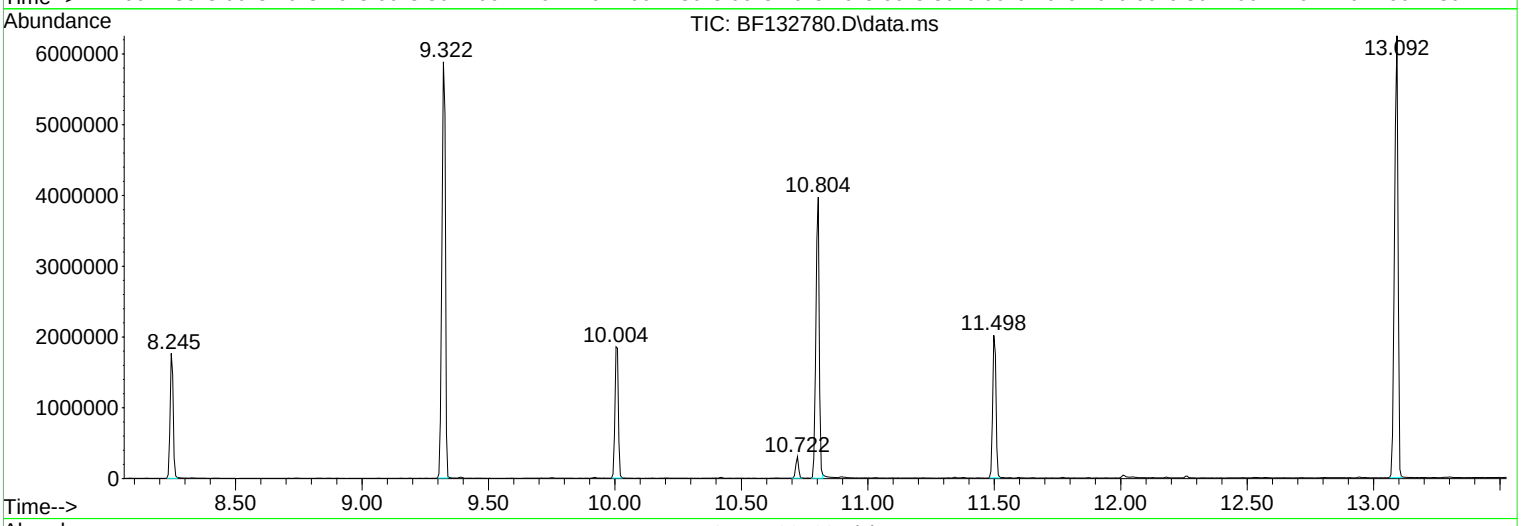
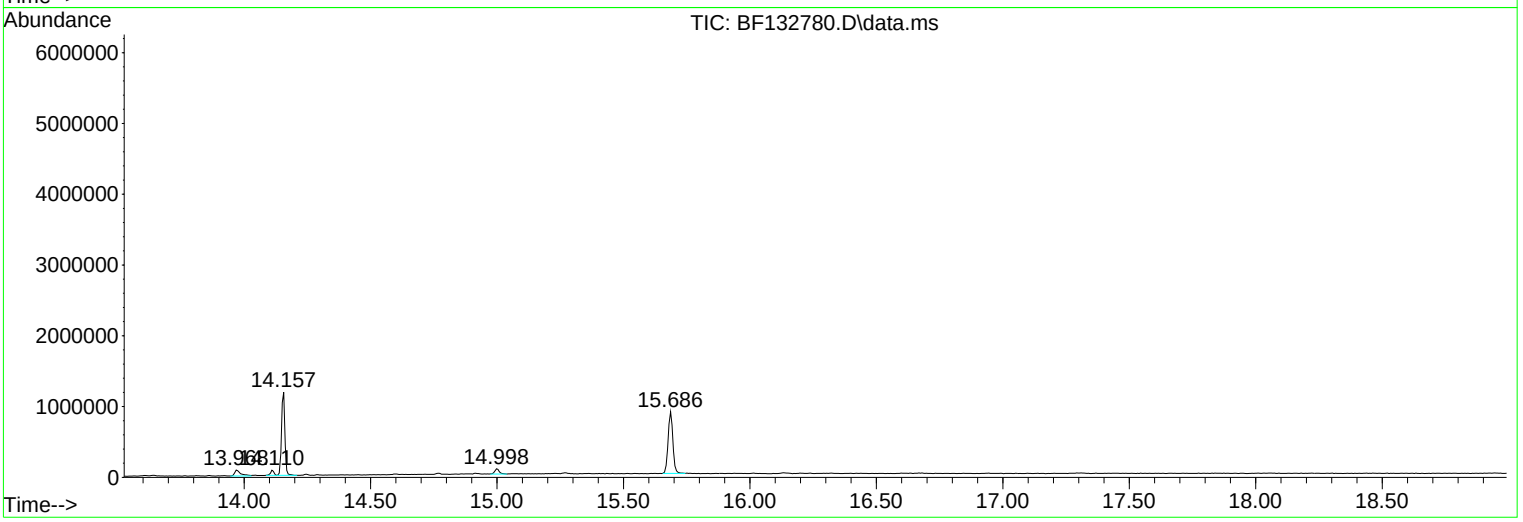
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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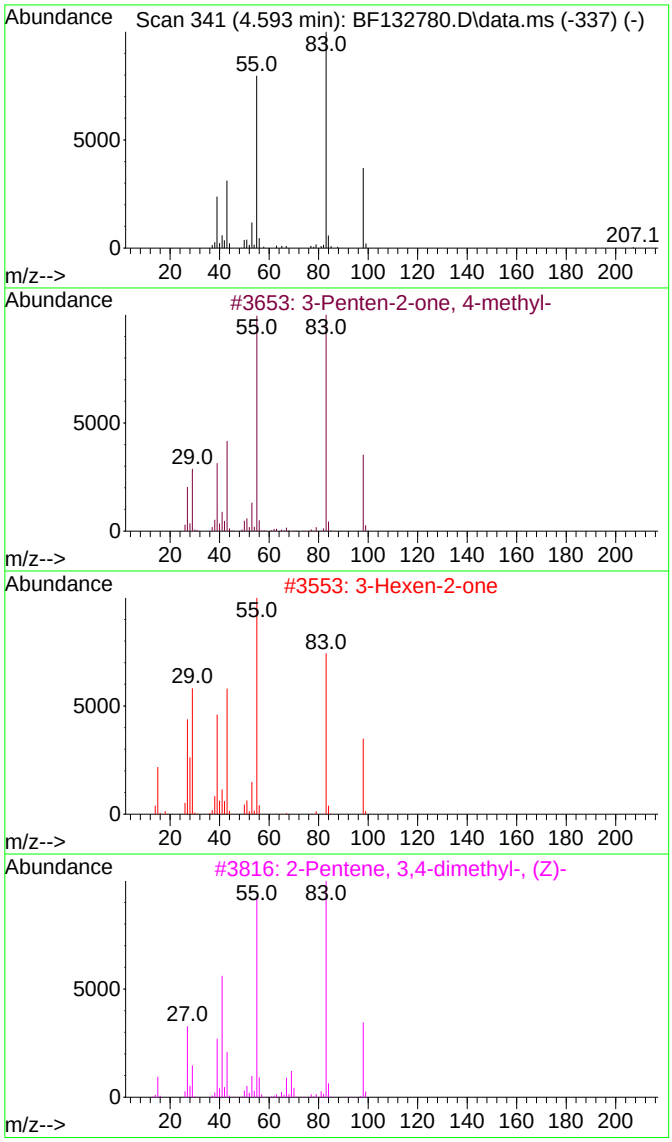
TIC Integration Parameters: LSCINT.P

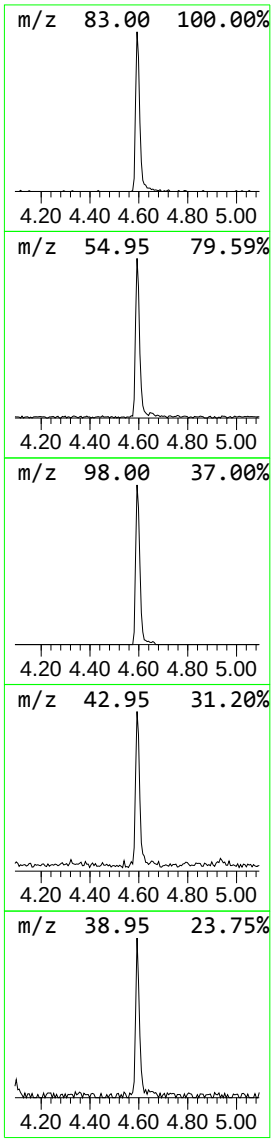
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.593	2.37 ng	136109	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





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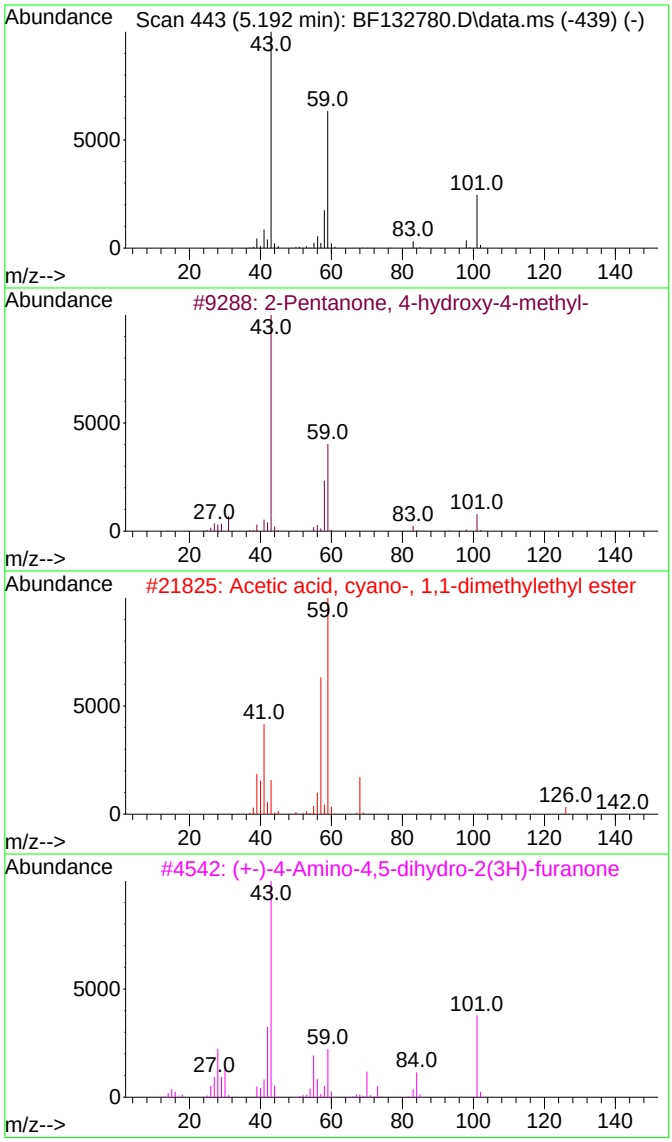
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

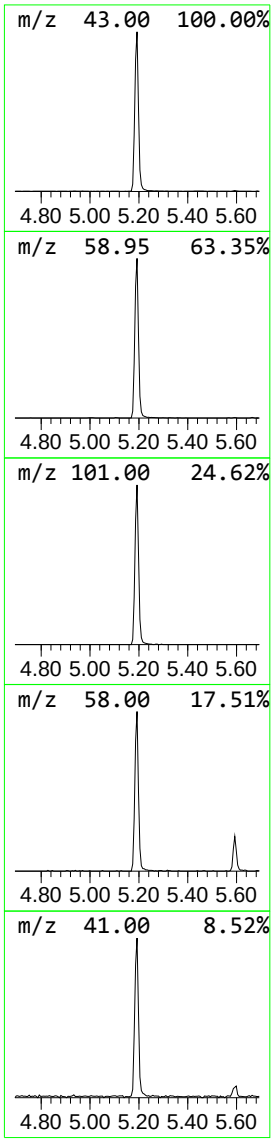
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	15.95 ng	917122	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





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BNA_F
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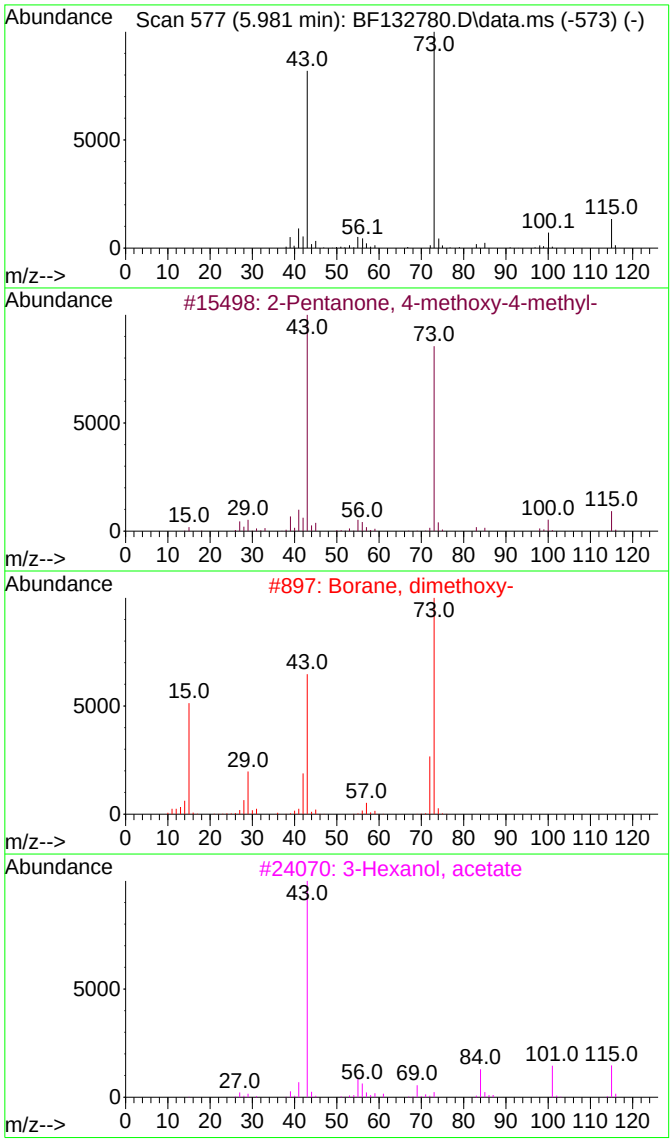
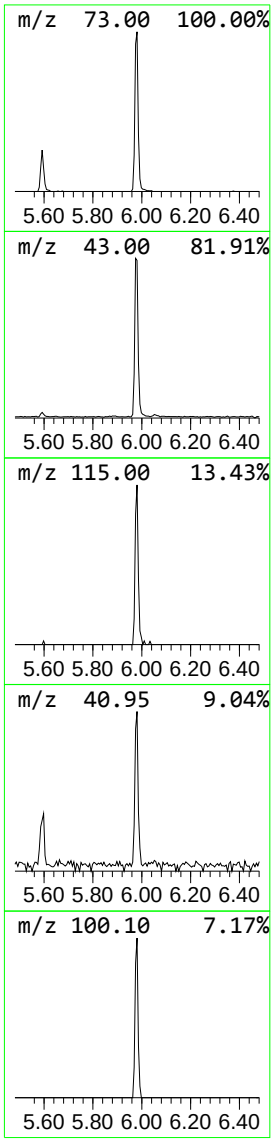
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	2.83 ng	162741	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	38
3	3-Hexanol, acetate	144	C8H16O2	040780-64-1	37
4	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
5	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23





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Instrument :
BNA_F
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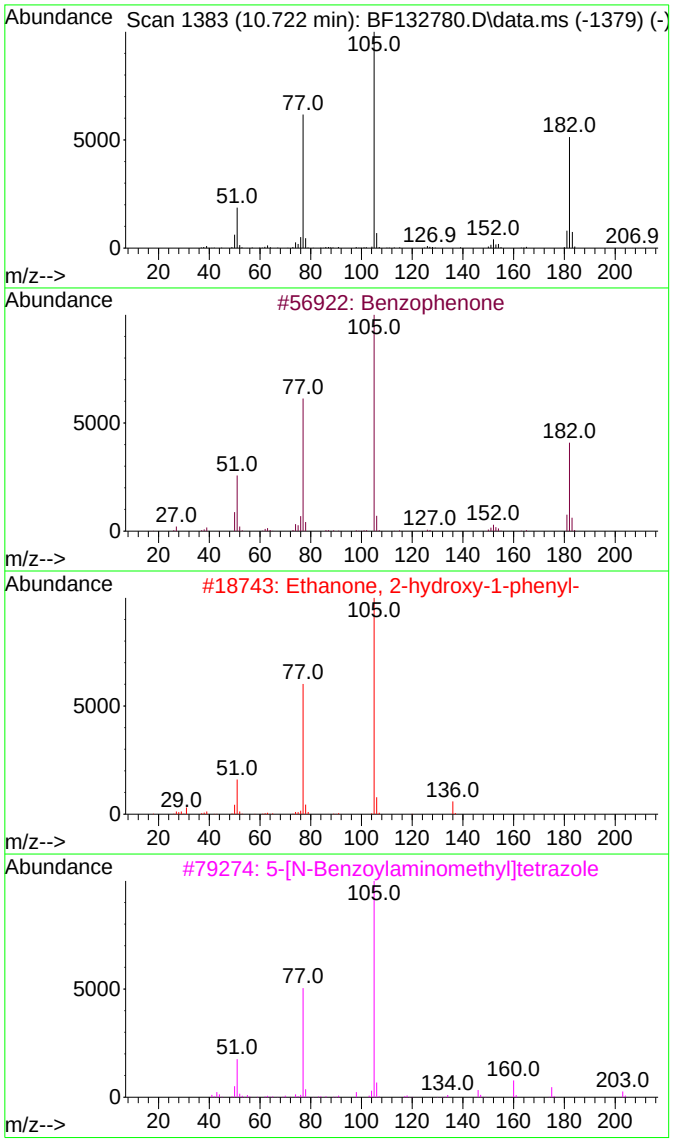
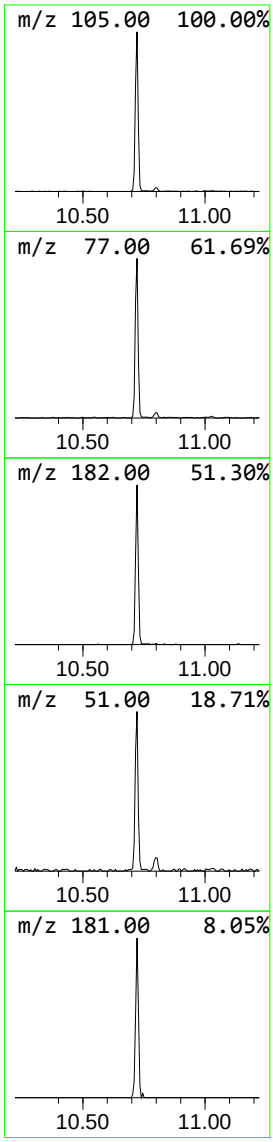
Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.722	2.74 ng	236771	Acenaphthene-d10	10.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	43
3	5-[N-Benzoylaminomethyl]tetrazole	203	C9H9N5O	1000227-36-3	43
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
5	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	43





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ClientSampleId :
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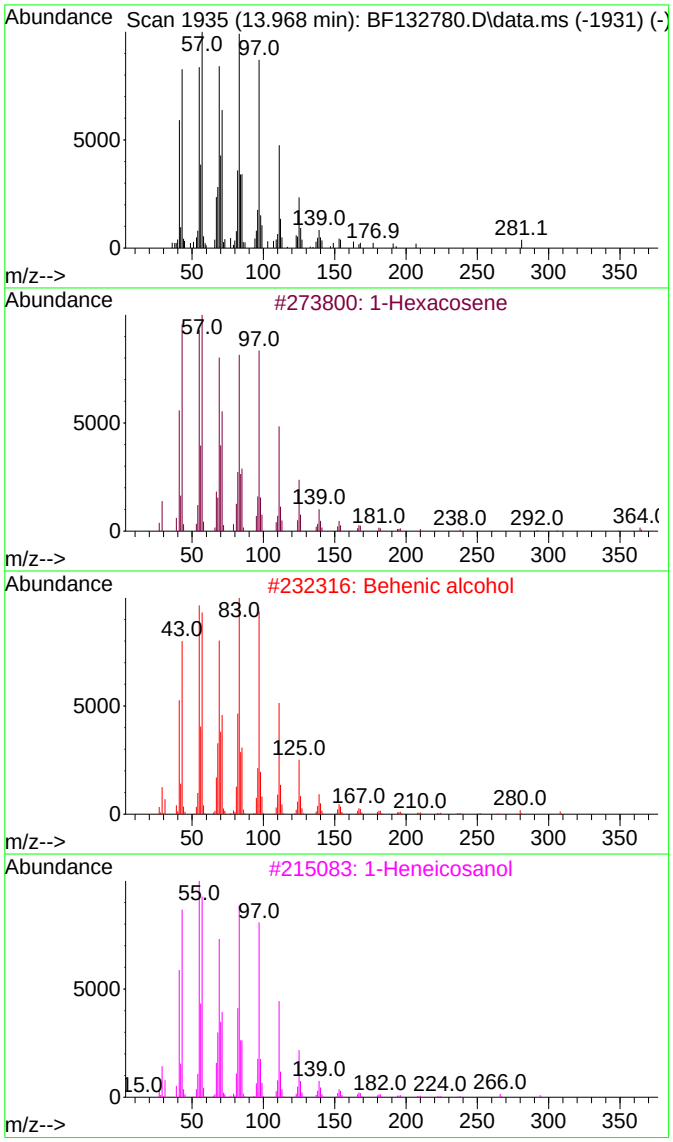
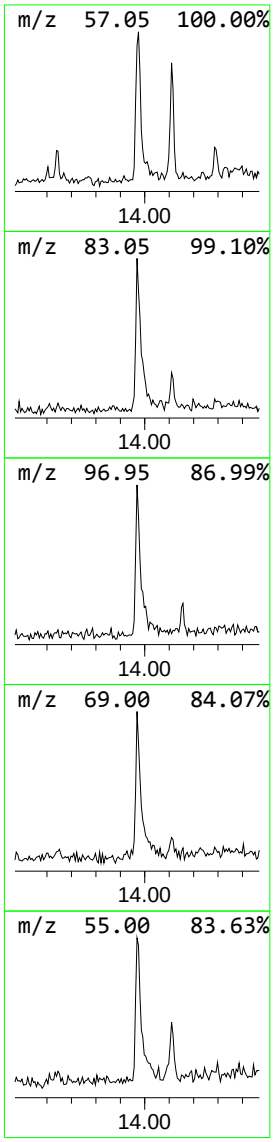
Peak Number 5 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.968	2.57 ng	139325	Chrysene-d12	14.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.593	2.4	ng	136109	1	6.963	1149900	20.0
2-Pentanone, 4-...	5.192	15.9	ng	917122	1	6.963	1149900	20.0
2-Pentanone, 4-...	5.981	2.8	ng	162741	1	6.963	1149900	20.0
Benzophenone	10.722	2.7	ng	236771	3	10.004	1729200	20.0
1-Hexacosene	13.968	2.6	ng	139325	5	14.157	1084000	20.0