

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
 Data File : BF099981.D
 Acq On : 31 Oct 2017 1:37
 Operator : SJ/JU
 Sample : I6083-07
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 102017-TIFR-F-D-S

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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.998	492	495	518	rBV	51233	80591	3.43%	0.566%
2	5.410	562	565	598	rBV	445016	660303	28.08%	4.637%
3	6.434	736	739	757	rBV	276329	427880	18.20%	3.005%
4	6.557	757	760	771	rVB	1348559	1249590	53.15%	8.776%
5	6.787	796	799	812	rVB	561873	492337	20.94%	3.458%
6	6.940	822	825	846	rVB	1789010	1698141	72.22%	11.926%
7	7.357	892	896	917	rBV	1260906	1263797	53.75%	8.875%
8	8.069	1014	1017	1036	rBV	774536	661006	28.11%	4.642%
9	8.628	1110	1112	1121	rBV	31067	33212	1.41%	0.233%
10	9.145	1196	1200	1203	rBV	2739772	2351236	100.00%	16.512%
11	9.539	1265	1267	1279	rBB	54371	52423	2.23%	0.368%
12	9.804	1309	1312	1313	rBV	44037	34102	1.45%	0.239%
13	9.822	1313	1315	1330	rVB	737825	700249	29.78%	4.918%
14	10.492	1427	1429	1434	rBB	44586	36945	1.57%	0.259%
15	10.539	1434	1437	1443	rBV	201289	155703	6.62%	1.093%
16	10.622	1447	1451	1465	rBV	888359	828162	35.22%	5.816%
17	11.316	1566	1569	1579	rBV	670839	638161	27.14%	4.482%
18	12.904	1835	1839	1843	rBV	1934412	1925012	81.87%	13.519%
19	13.786	1986	1989	1998	rBV	40427	56293	2.39%	0.395%
20	13.980	2018	2022	2031	rVB	492443	468595	19.93%	3.291%
21	15.474	2272	2276	2287	rVB	319922	425431	18.09%	2.988%

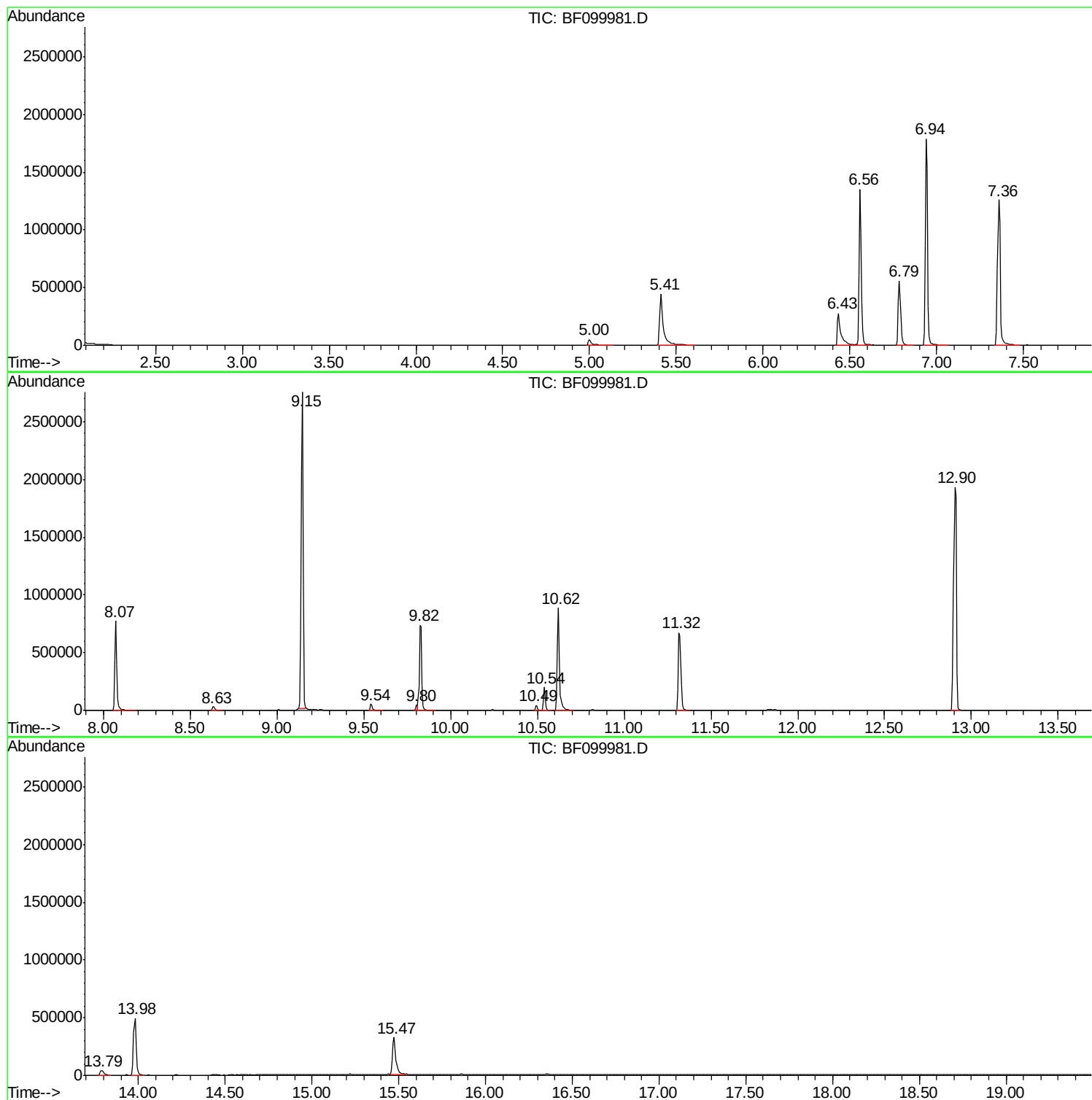
Sum of corrected areas: 14239169

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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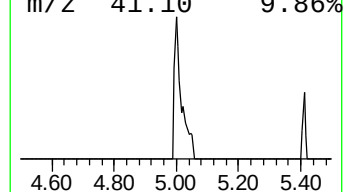
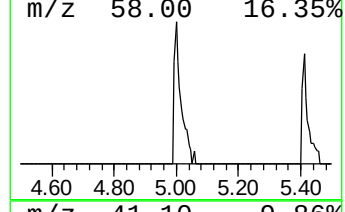
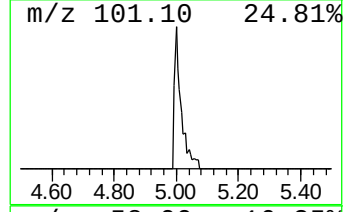
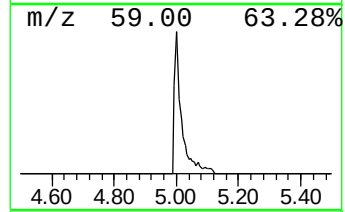
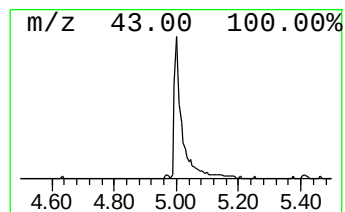
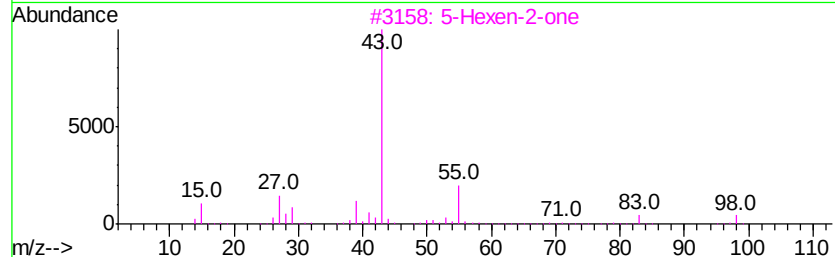
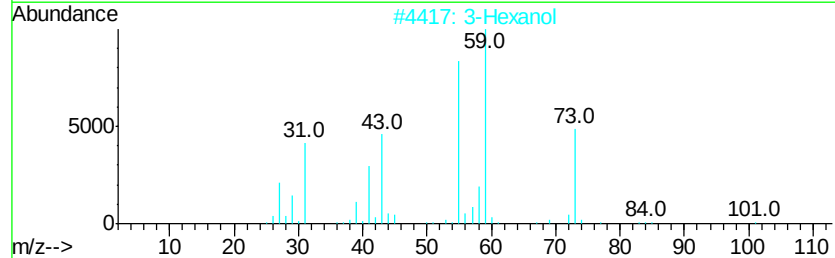
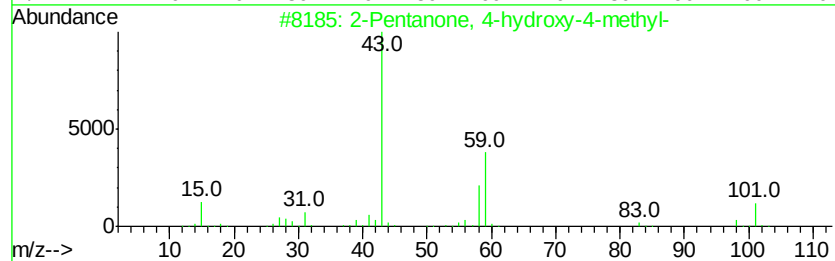
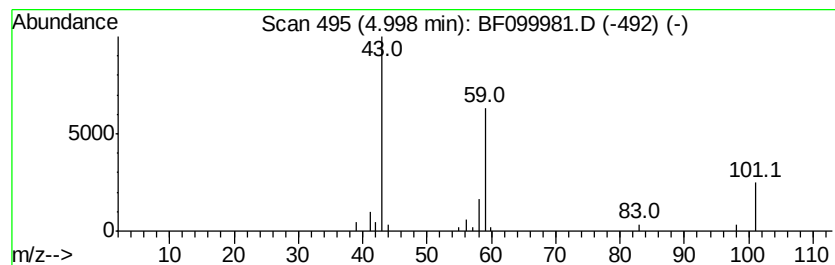
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.27 ng	80591	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Hexanol	102	C6H14O	000623-37-0	28
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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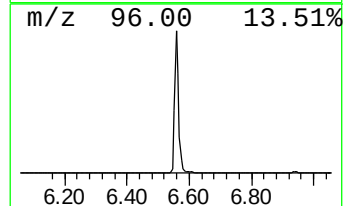
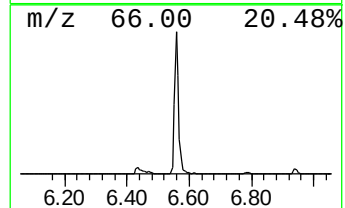
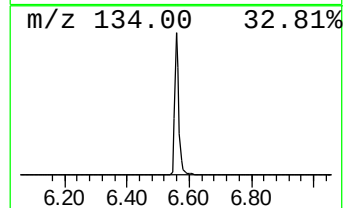
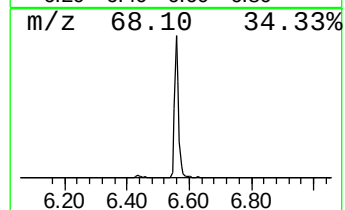
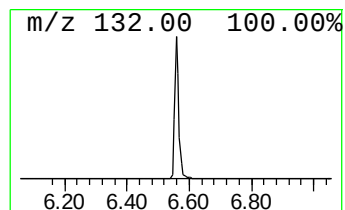
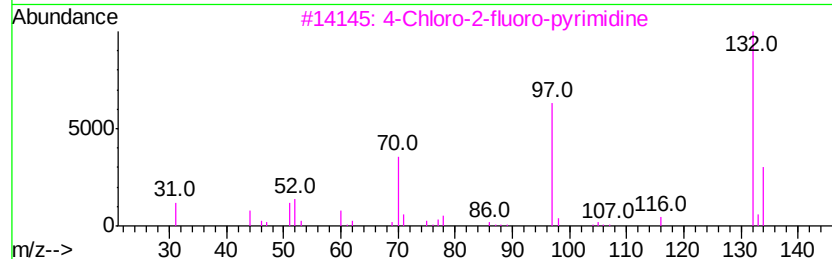
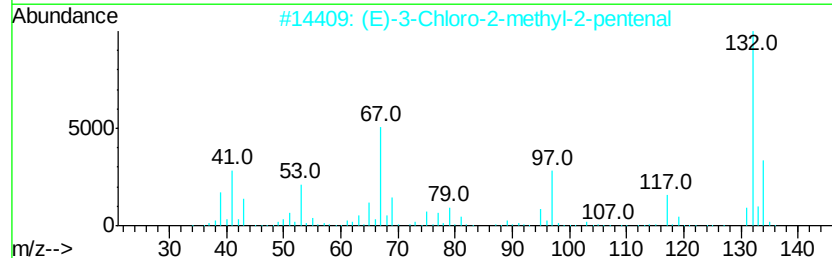
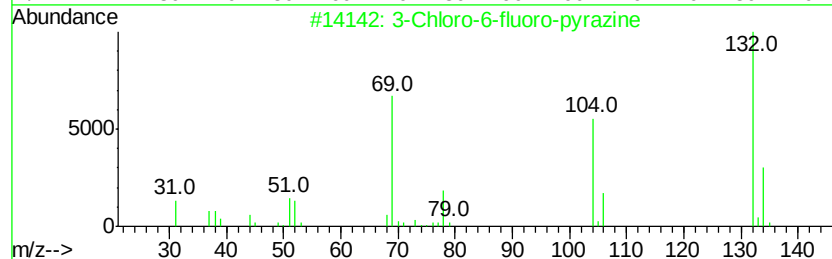
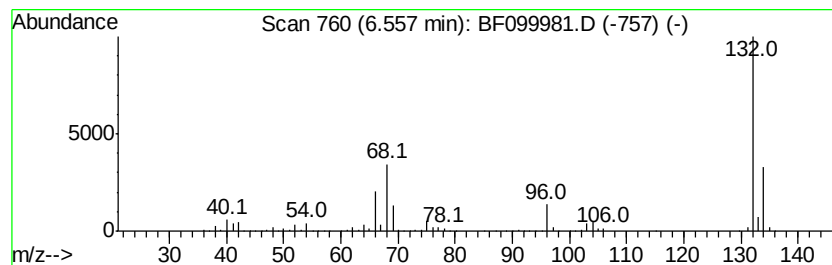
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Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	50.76 ng	1249590	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		1-Aminoindan	133	C9H11N	034698-41-4	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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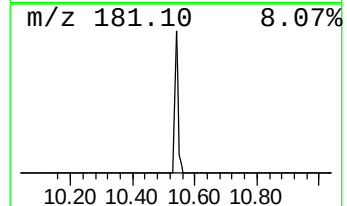
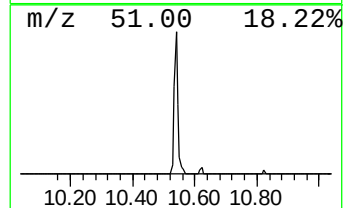
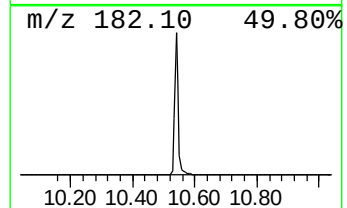
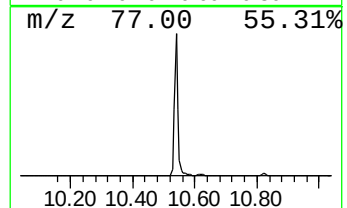
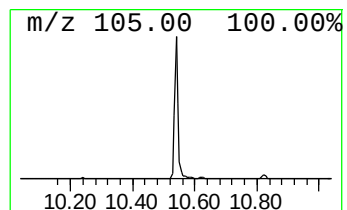
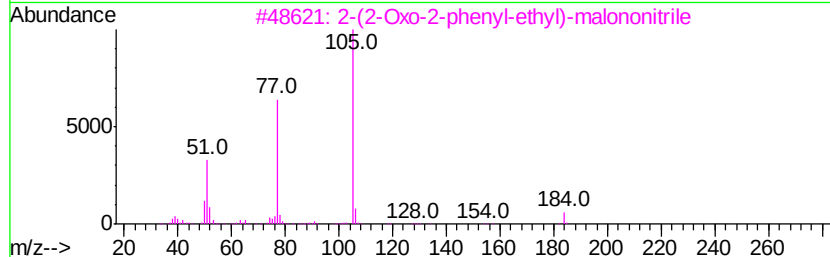
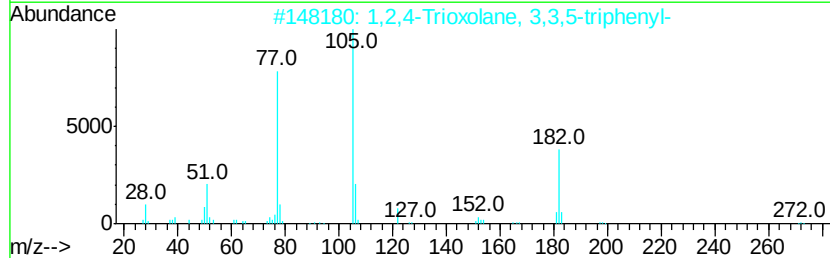
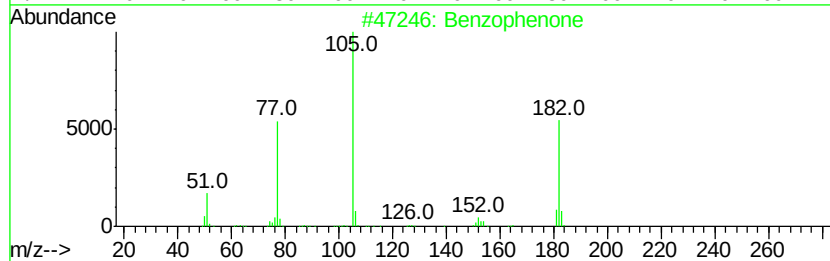
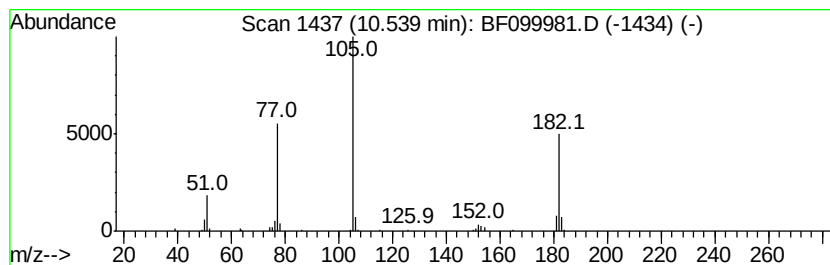
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Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	4.45 ng	155703	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3		2-(2-Oxo-2-phenyl-ethyl)-malononitrile	184	C11H8N2O	1000296-76-9	47
4		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	46
5		3-Deoxy-L-ribose-2,5-dibenzoate	342	C19H18O6	1000194-12-7	43



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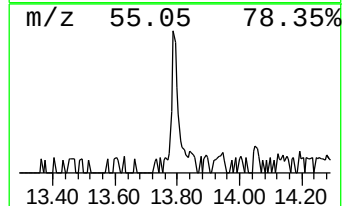
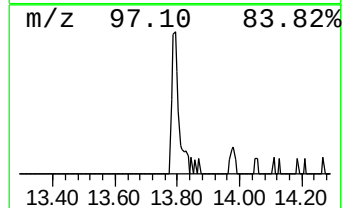
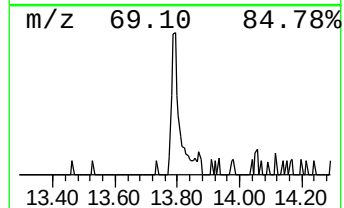
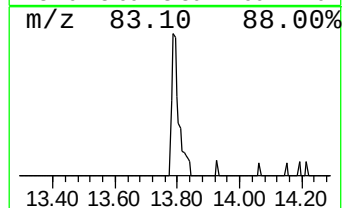
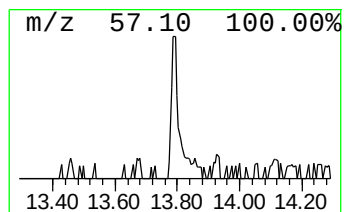
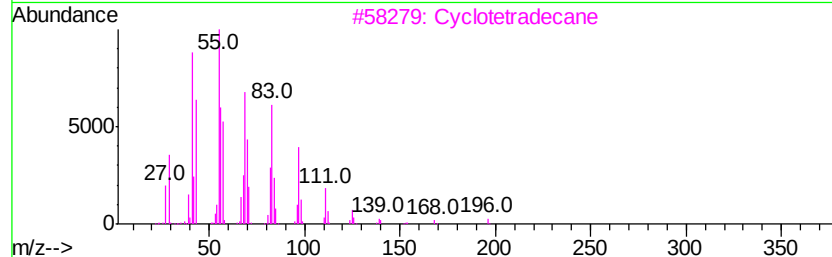
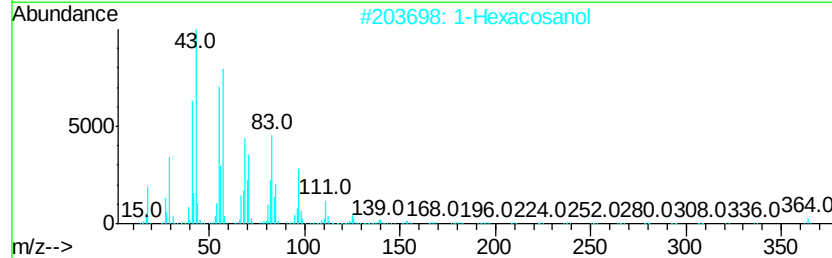
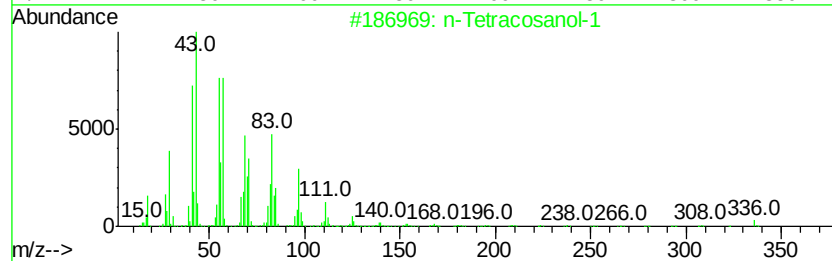
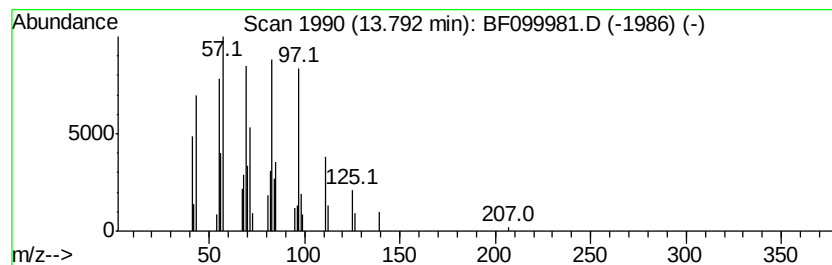
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Peak Number 5 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.40 ng	56293	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	81
2		1-Hexacosanol	382	C26H54O	000506-52-5	74
3		Cyclotetradecane	196	C14H28	000295-17-0	68
4		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	58
5		Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	3.3	ng	80591	1	6.79	492337	20.0
unknown6.56	6.56	50.8	ng	1249590	1	6.79	492337	20.0
Benzophenone	10.54	4.5	ng	155703	3	9.82	700249	20.0
n-Tetracosanol-1	13.79	2.4	ng	56293	5	13.98	468595	20.0