

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
 Data File : BF100831.D
 Acq On : 22 Nov 2017 19:00
 Operator : SJ/JU
 Sample : PB104479BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB104479BL

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-BF110817.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	5.098	507	512	523	rBV	205780	304336	11.38%	1.496%
2	5.487	573	578	581	rBV	1946947	2084120	77.92%	10.245%
3	6.492	743	749	752	rBV	1898799	2041548	76.33%	10.036%
4	6.634	768	773	776	rBV	2181695	2131298	79.68%	10.477%
5	6.857	808	811	815	rVB	530856	454587	17.00%	2.235%
6	7.016	834	838	841	rBV	1855745	1705061	63.75%	8.382%
7	7.422	901	907	910	rBV	1177198	1349520	50.45%	6.634%
8	8.139	1024	1029	1033	rBV	689496	616509	23.05%	3.031%
9	9.222	1206	1213	1216	rBV	2542154	2674750	100.00%	13.149%
10	9.898	1323	1328	1331	rBV	798505	706717	26.42%	3.474%
11	10.310	1393	1398	1403	rVB	26667	39038	1.46%	0.192%
12	10.692	1457	1463	1466	rBV	1479175	1560580	58.34%	7.672%
13	11.386	1577	1581	1584	rBV	898472	763162	28.53%	3.752%
14	12.686	1797	1802	1806	rBV3	19916	31224	1.17%	0.153%
15	12.974	1845	1851	1854	rBV	2587086	2624136	98.11%	12.900%
16	13.886	2003	2006	2010	rVB	67321	62310	2.33%	0.306%
17	13.992	2017	2024	2025	rBV5	18776	27339	1.02%	0.134%
18	14.021	2025	2029	2033	rVB	621692	574105	21.46%	2.822%
19	14.862	2168	2172	2178	rVB	70768	81717	3.06%	0.402%
20	15.398	2259	2263	2266	rBV	31844	36805	1.38%	0.181%
21	15.492	2274	2279	2287	rBV	368121	473352	17.70%	2.327%

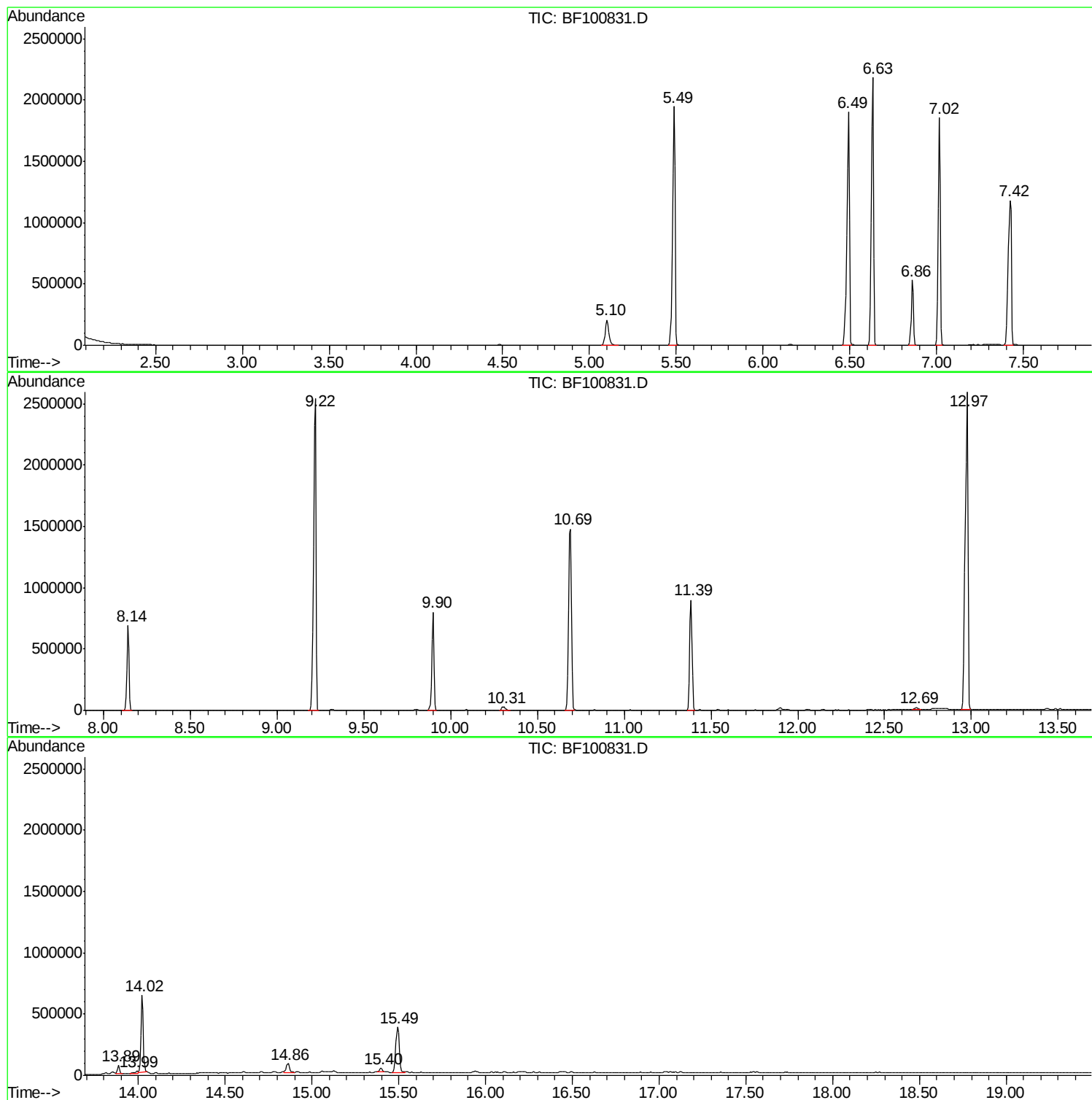
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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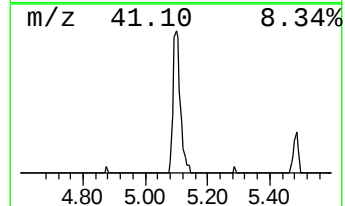
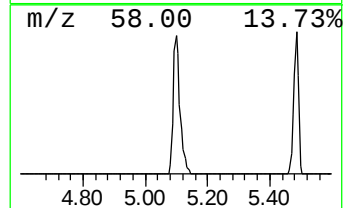
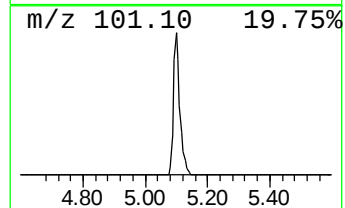
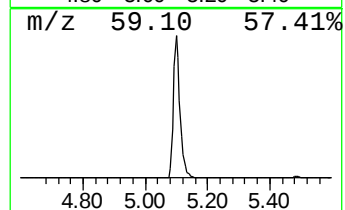
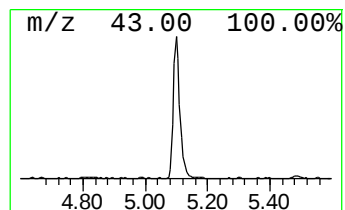
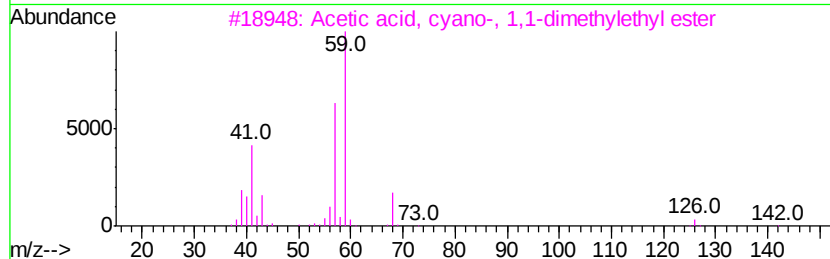
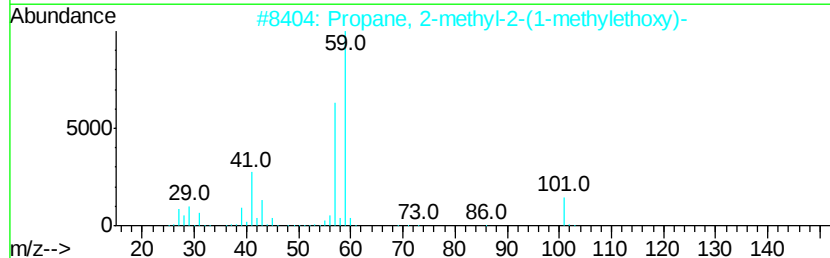
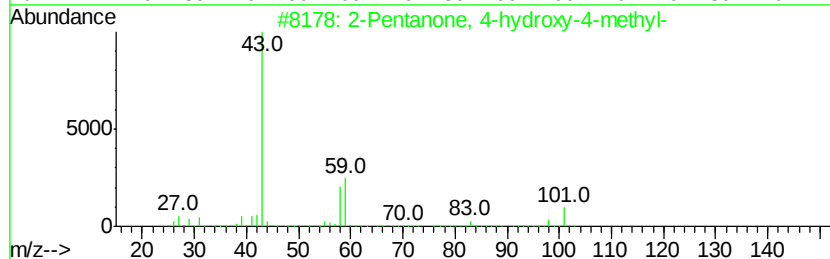
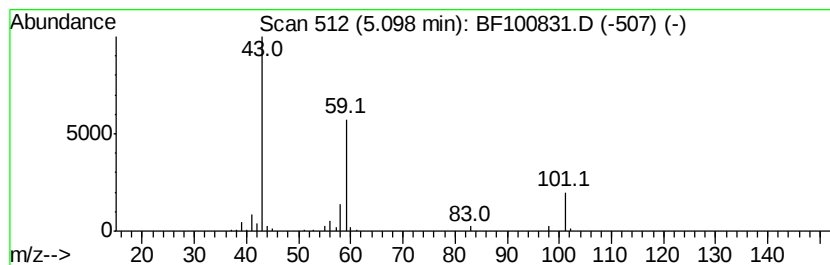
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	13.39 ng	304336	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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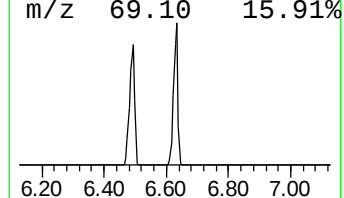
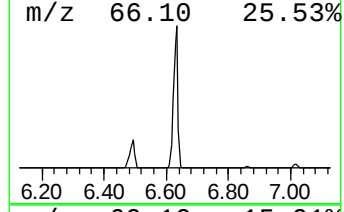
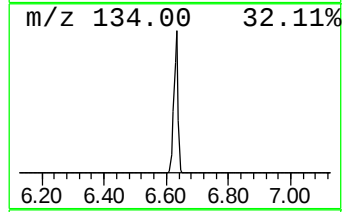
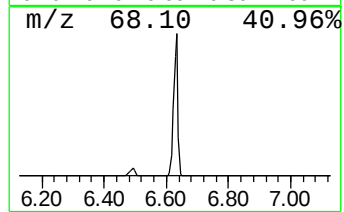
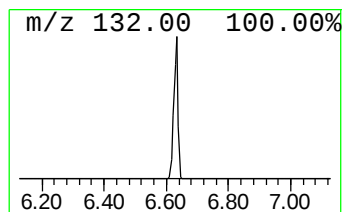
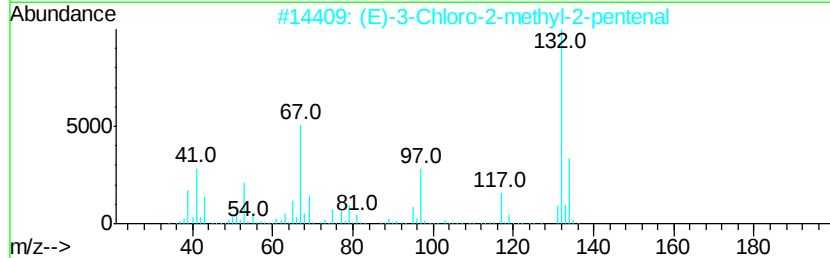
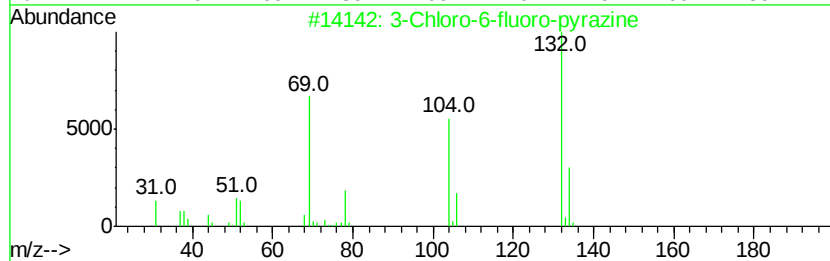
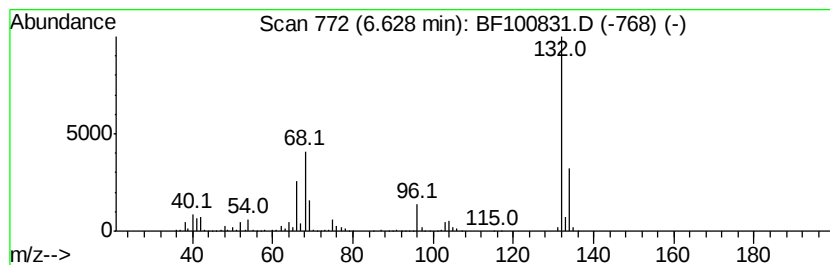
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	93.77 ng	2131300	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropane-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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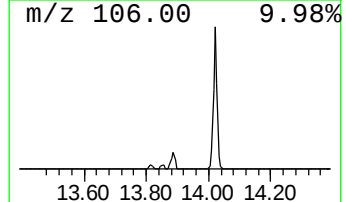
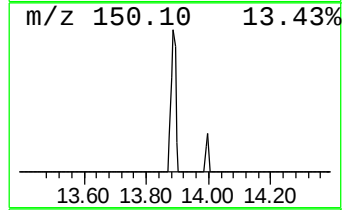
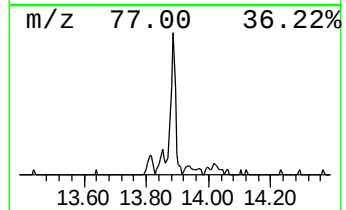
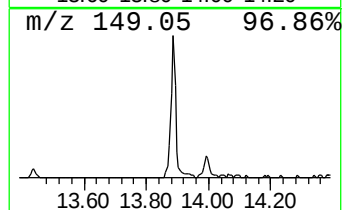
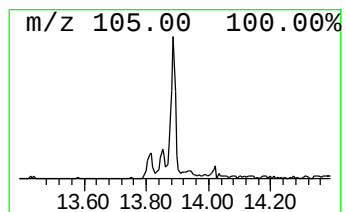
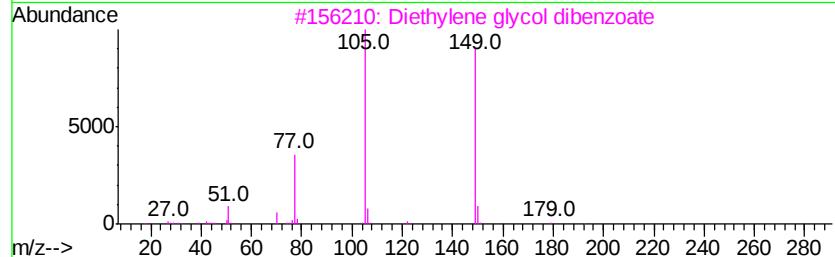
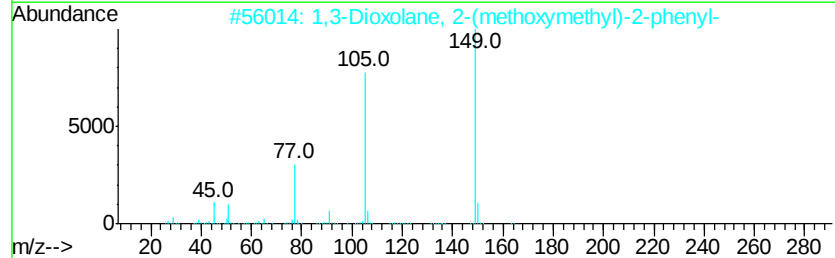
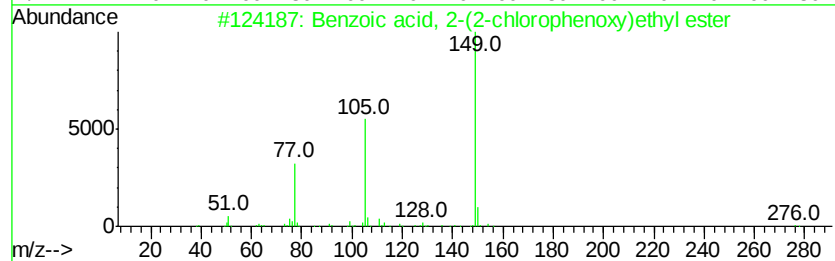
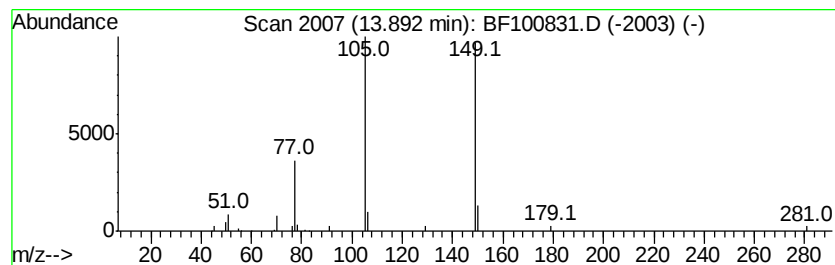
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Peak Number 4 Benzoic acid, 2-(2-chloroph... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.17 ng	62310	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	83
2		1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
3		Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
4		3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	83
5		Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78



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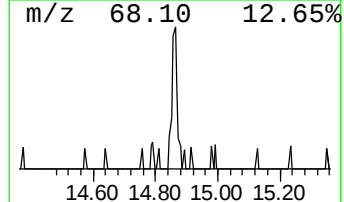
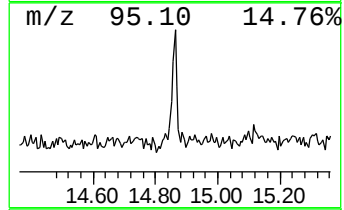
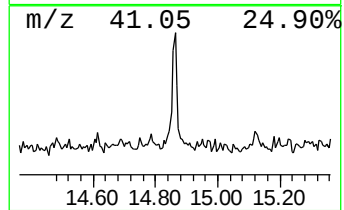
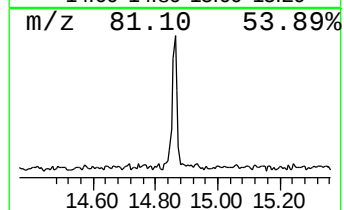
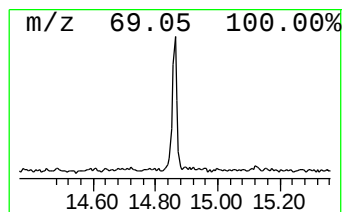
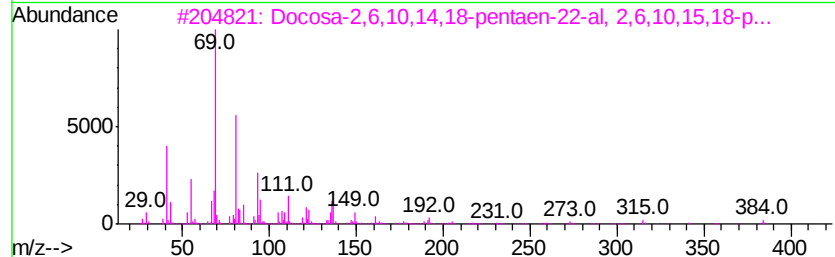
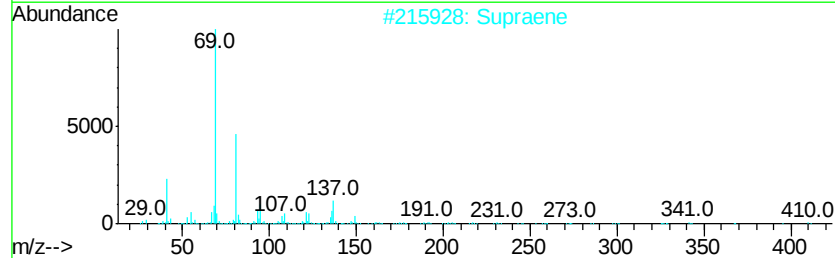
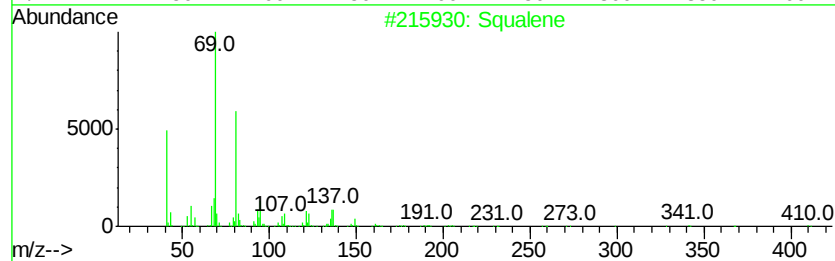
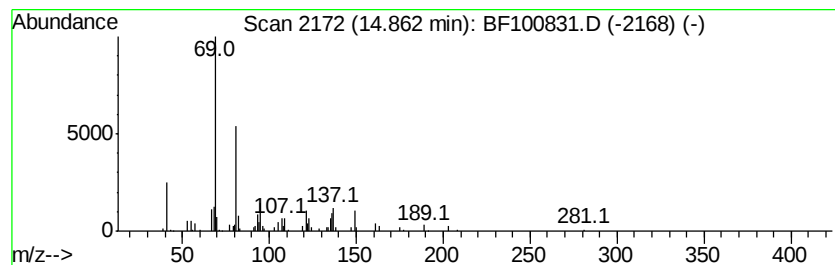
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	3.45 ng	81717	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	90
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	13.4	ng	304336	1	6.86	454587	20.0
unknown6.63	6.63	93.8	ng	2131300	1	6.86	454587	20.0
Benzoic acid, 2-(...	13.89	2.2	ng	62310	5	14.02	574105	20.0
Squalene	14.86	3.5	ng	81717	6	15.49	473352	20.0