

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
 Data File : BG027333.D
 Acq On : 9 Jun 2017 1:32
 Operator : SJ/MA
 Sample : I3479-10
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TW-7-20170604

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_G\METHODS\8270-BG060517.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	5.700	335	342	352	rBV	64853	108149	2.14%	0.479%
2	6.140	406	417	427	rBV	533621	921155	18.19%	4.078%
3	7.685	673	680	693	rVB	361690	675723	13.35%	2.992%
4	8.091	740	749	761	rBV	871178	1627137	32.14%	7.204%
5	8.555	822	828	839	rVB	160941	300145	5.93%	1.329%
6	8.884	876	884	895	rBV	675744	1245567	24.60%	5.515%
7	9.718	1017	1026	1033	rBV	627885	1204113	23.78%	5.331%
8	11.375	1299	1308	1314	rBV	256844	495116	9.78%	2.192%
9	13.761	1704	1714	1725	rBV	1911398	3113008	61.49%	13.783%
10	14.566	1845	1851	1857	rBV	87014	134897	2.66%	0.597%
11	15.136	1939	1948	1962	rBV2	555565	1002702	19.81%	4.439%
12	15.705	2037	2045	2053	rBV2	91887	150166	2.97%	0.665%
13	16.622	2193	2201	2211	rVB	1701765	2793463	55.18%	12.368%
14	17.885	2409	2416	2429	rVB2	603559	1002070	19.79%	4.437%
15	18.725	2554	2559	2569	rBV	110251	179860	3.55%	0.796%
16	19.983	2768	2773	2781	rBV2	88688	132713	2.62%	0.588%
17	20.465	2848	2855	2861	rBV	3714467	5062700	100.00%	22.415%
18	21.828	3083	3087	3098	rVB3	44357	81594	1.61%	0.361%
19	22.274	3155	3163	3172	rVB	597190	1160197	22.92%	5.137%
20	23.156	3308	3313	3319	rBV9	37822	79652	1.57%	0.353%
21	25.958	3779	3790	3806	rVB2	340106	1115993	22.04%	4.941%

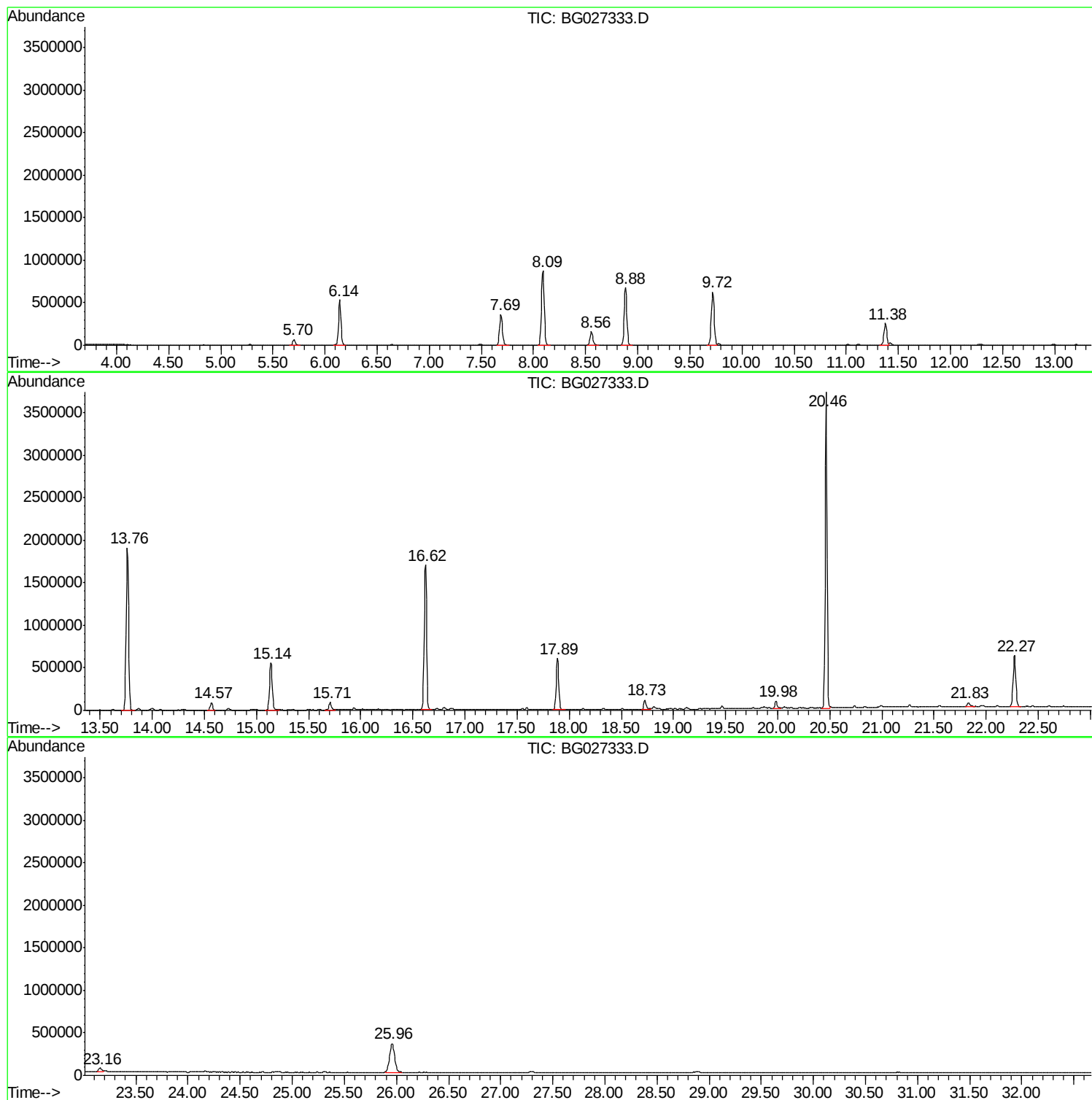
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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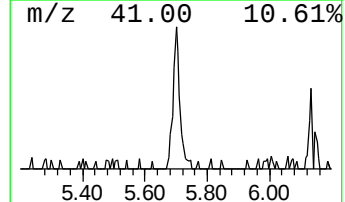
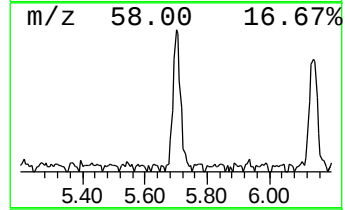
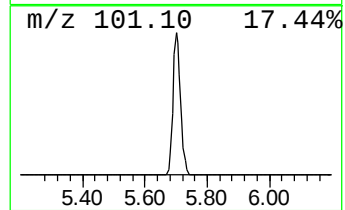
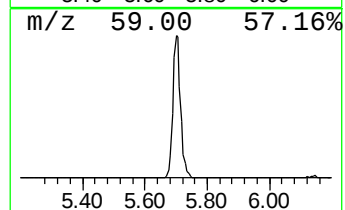
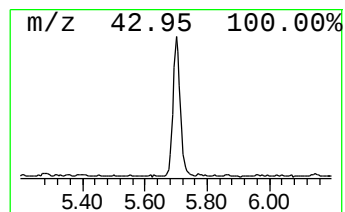
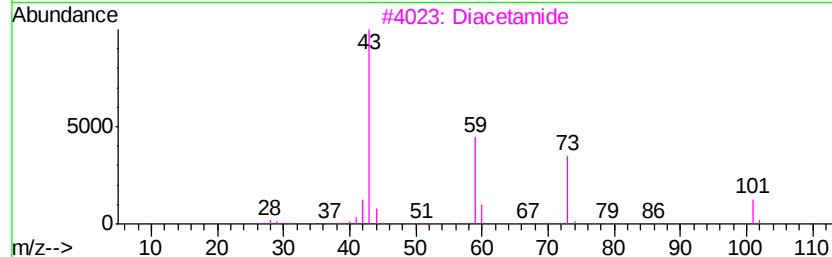
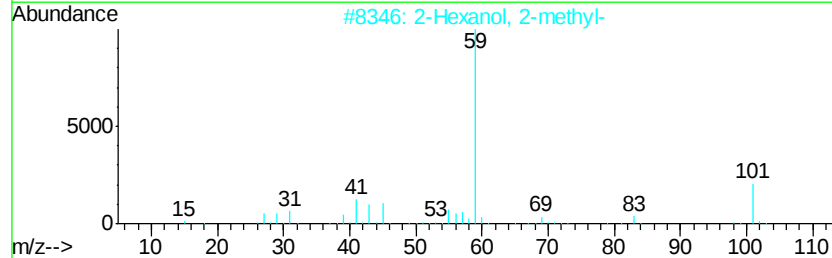
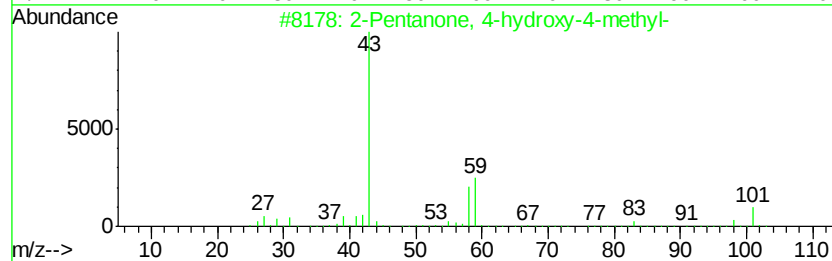
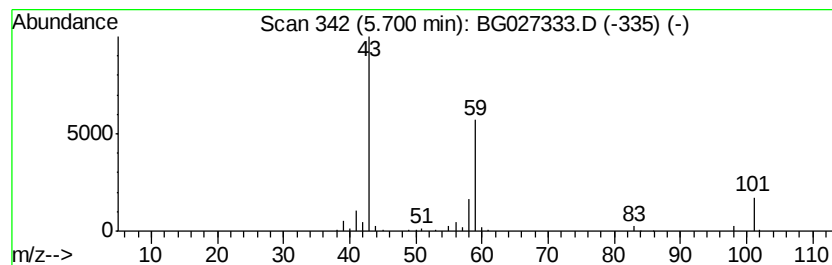
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.70	7.21 ng	108149	1,4-Dichlorobenzene-d4	8.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
3	Diacetamide	101	C4H7NO2	000625-77-4	9	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9	



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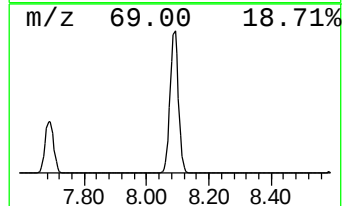
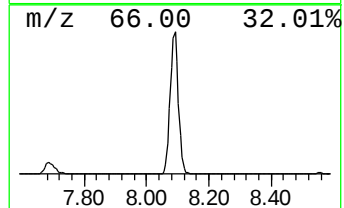
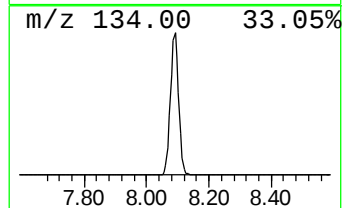
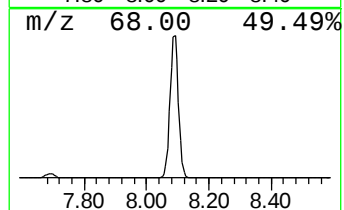
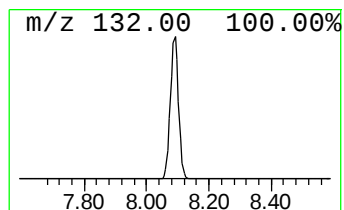
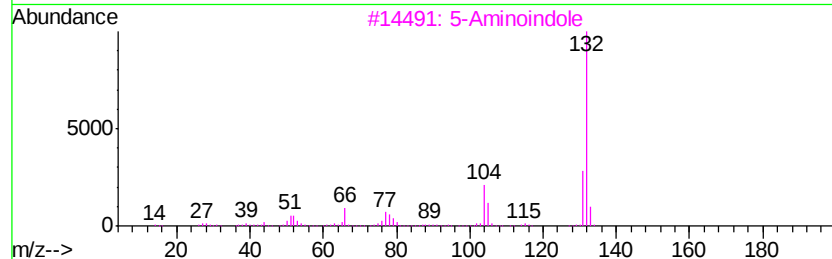
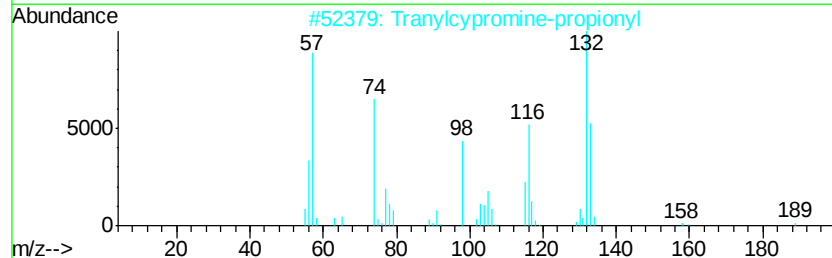
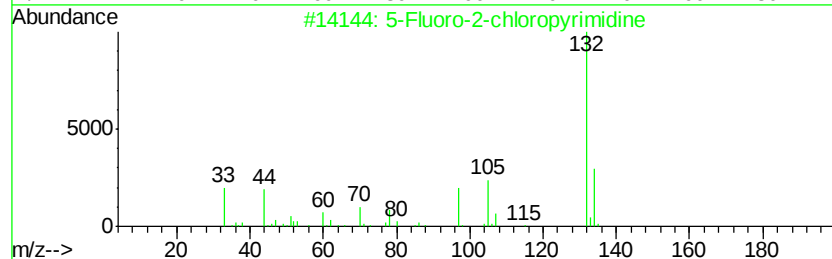
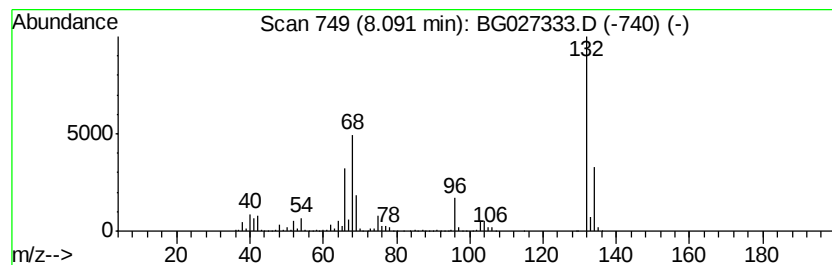
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown8.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	108.42 ng	1627140	1,4-Dichlorobenzene-d4	8.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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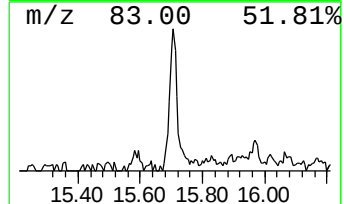
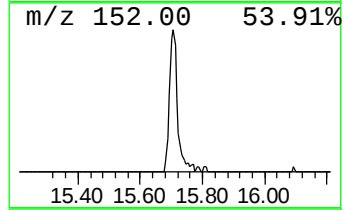
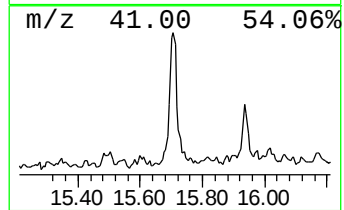
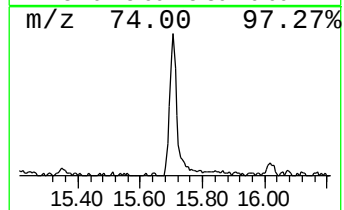
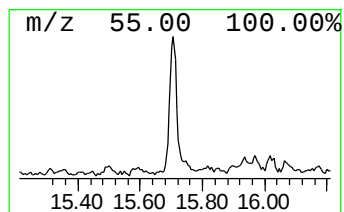
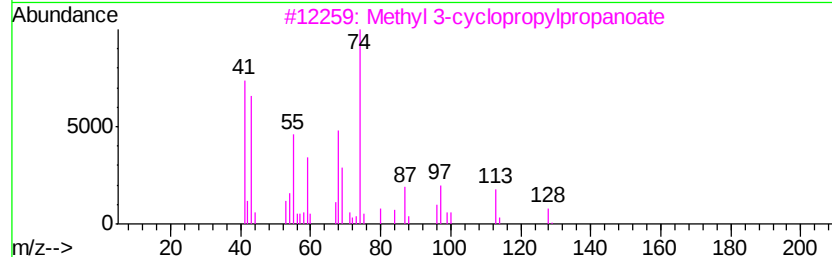
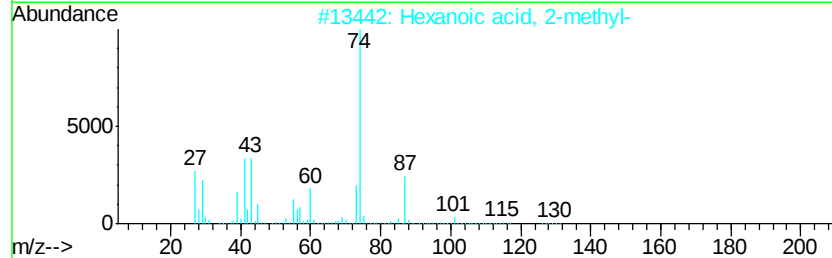
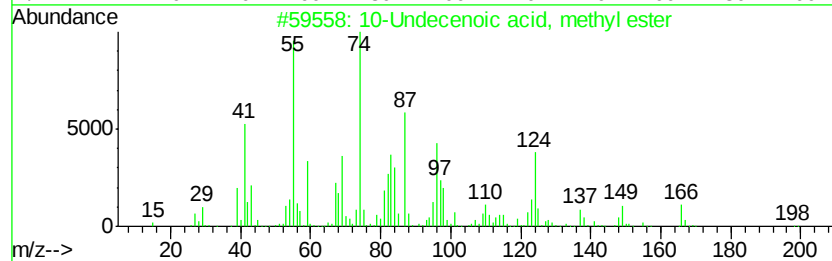
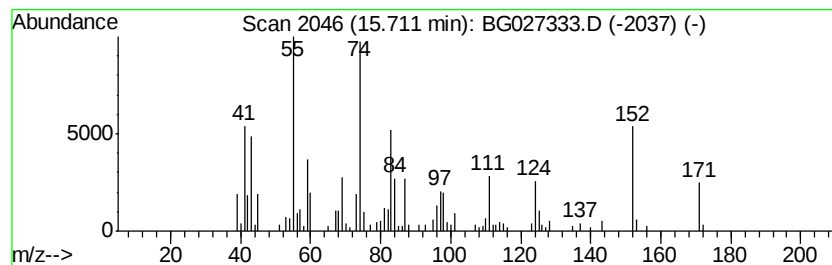
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Peak Number 4 unknown15.71 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.00 ng	150166	Acenaphthene-d10	15.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Undecenoic acid, methyl ester	198	C12H22O2	000111-81-9	47	
2	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	27	
3	Methyl 3-cyclopropylpropanoate	128	C7H12O2	062021-34-5	27	
4	5-Hexenoic acid, methyl ester	128	C7H12O2	002396-80-7	25	
5	Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	22	



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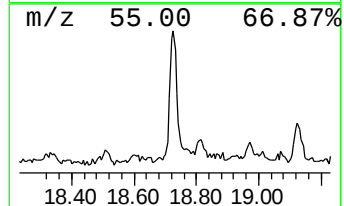
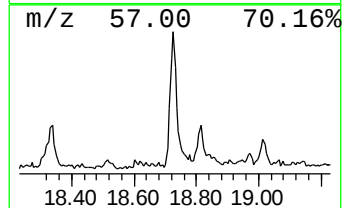
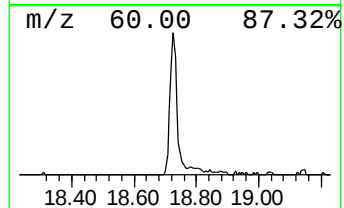
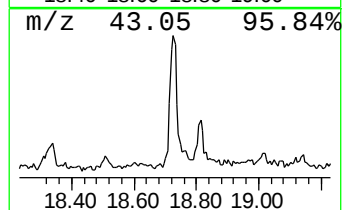
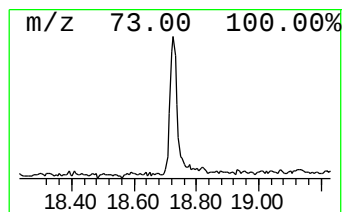
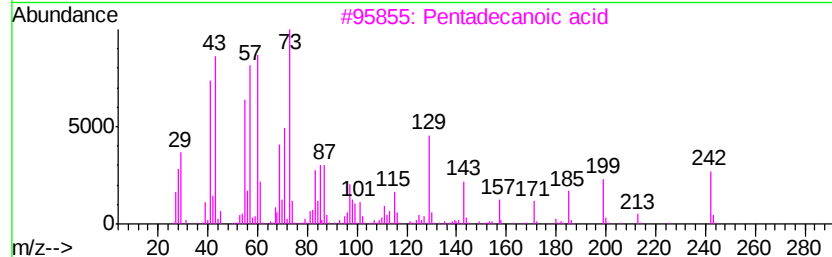
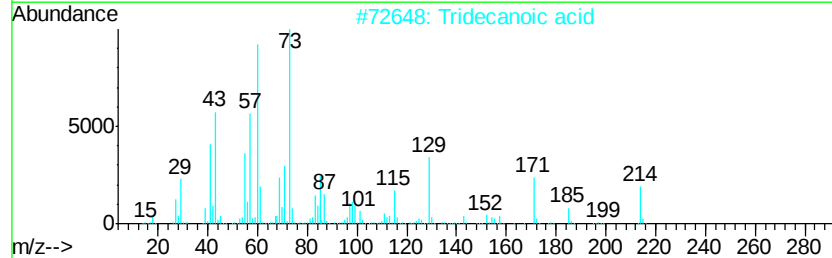
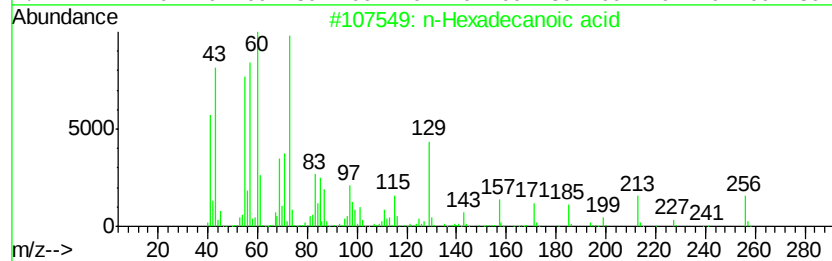
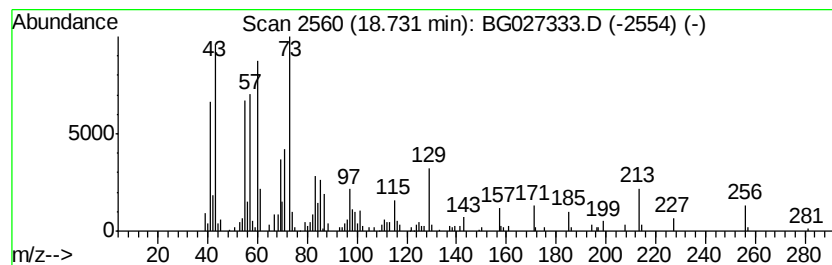
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.73	3.59 ng	179860	Phenanthrene-d10	17.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Estra-1,3,5(10)-trien-17.β-ol	256	C18H24O	002529-64-8	30



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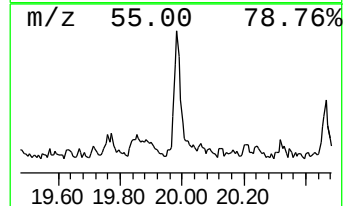
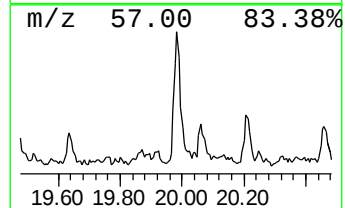
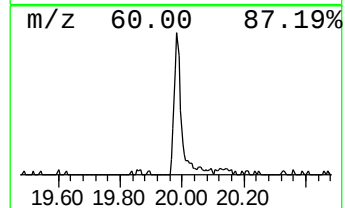
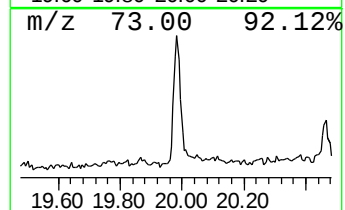
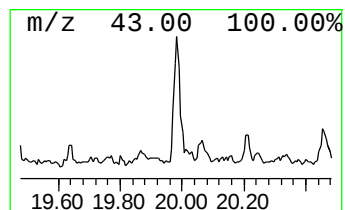
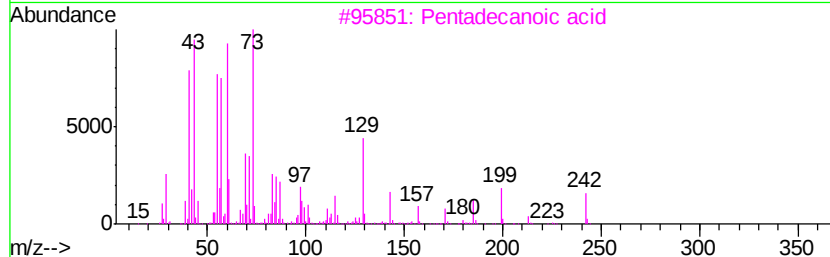
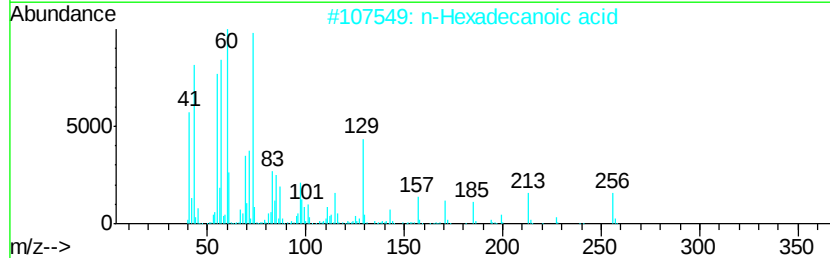
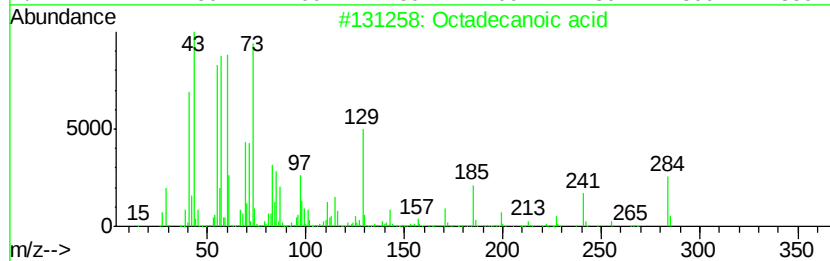
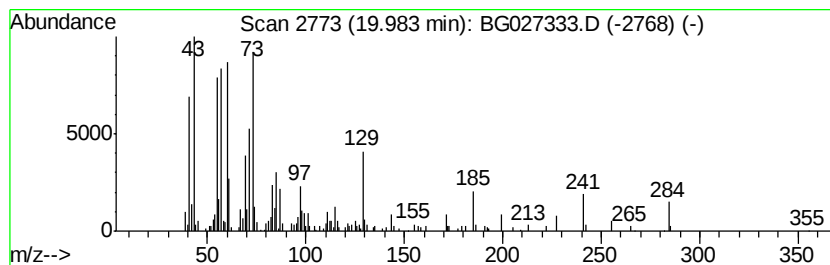
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Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.98	2.65 ng	132713	Phenanthrene-d10	17.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.70	7.2	ng	108149	1	8.56	300145	20.0
unknown8.09	8.09	108.4	ng	1627140	1	8.56	300145	20.0
unknown15.71	15.71	3.0	ng	150166	3	15.14	1002700	20.0
n-Hexadecanoic acid	18.73	3.6	ng	179860	4	17.89	1002070	20.0
Octadecanoic acid	19.98	2.6	ng	132713	4	17.89	1002070	20.0