

Data Path : Z:\HPCHEM1\BNA G\Data\BG032517\
 Data File : BG026424.D
 Acq On : 24 Mar 2017 21:09
 Operator : SJ/MA
 Sample : I2378-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 25A-7-9

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-BG032017.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	5.140	342	349	360	rBV	285497	449199	4.46%	0.839%
2	5.616	423	430	444	rBV	2255202	3615301	35.92%	6.755%
3	7.209	693	701	719	rBV	2241410	3850075	38.25%	7.193%
4	7.579	756	764	773	rBV	2419185	4127024	41.01%	7.711%
5	8.043	836	843	850	rBV	449336	750433	7.46%	1.402%
6	8.366	890	898	906	rBV	2001422	3409094	33.87%	6.369%
7	9.200	1032	1040	1050	rBV	1383995	2437520	24.22%	4.554%
8	10.846	1312	1320	1333	rBV	601845	1107834	11.01%	2.070%
9	13.278	1725	1734	1741	rBV	4096931	6474439	64.33%	12.096%
10	14.095	1866	1873	1884	rBV	517836	767573	7.63%	1.434%
11	14.647	1960	1967	1977	rBV2	913621	1513925	15.04%	2.829%
12	16.128	2212	2219	2236	rBV	2934726	4471363	44.43%	8.354%
13	17.379	2425	2432	2440	rBV	1323927	1985362	19.73%	3.709%
14	18.255	2576	2581	2590	rBV	346588	532967	5.30%	0.996%
15	19.112	2723	2727	2735	rBV2	73219	148222	1.47%	0.277%
16	19.524	2792	2797	2804	rBV	158793	256964	2.55%	0.480%
17	19.982	2868	2875	2881	rBV	7343021	10064315	100.00%	18.804%
18	21.269	3089	3094	3112	rBV2	288922	600588	5.97%	1.122%
19	21.504	3131	3134	3139	rVB2	81541	118625	1.18%	0.222%
20	21.627	3148	3155	3165	rBV	1654687	2653621	26.37%	4.958%
21	22.144	3237	3243	3261	rVB4	98928	325794	3.24%	0.609%
22	22.773	3344	3350	3365	rVB	702557	1195737	11.88%	2.234%
23	24.806	3685	3696	3709	rBV2	930076	2667628	26.51%	4.984%

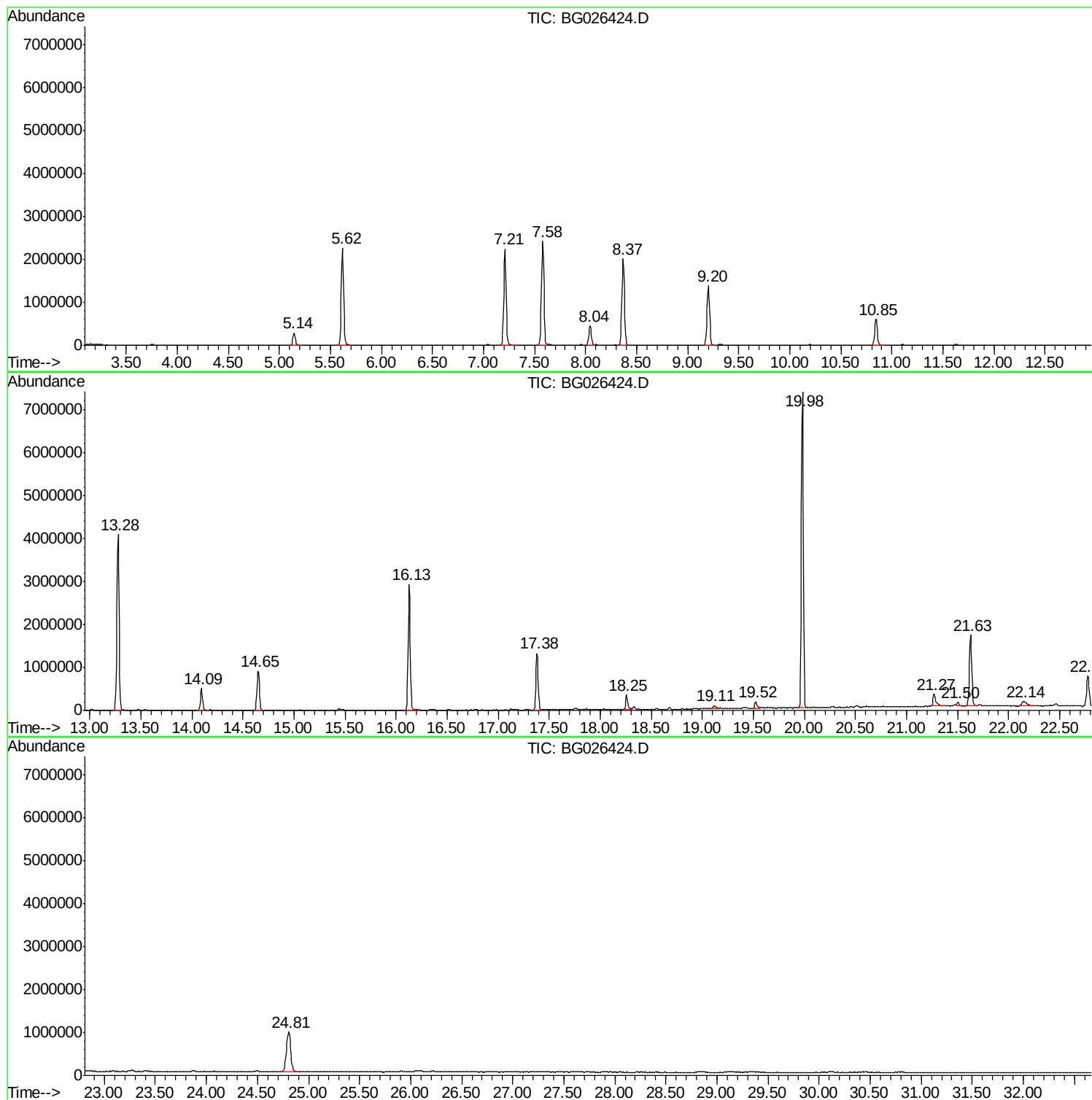
Sum of corrected areas: 53523603

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG032017.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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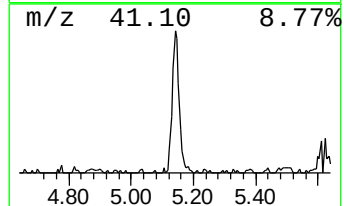
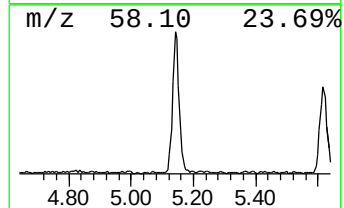
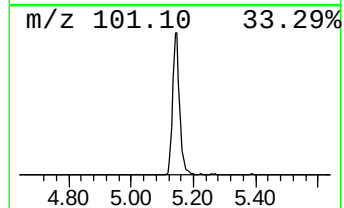
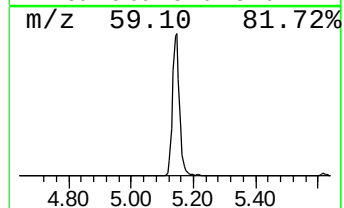
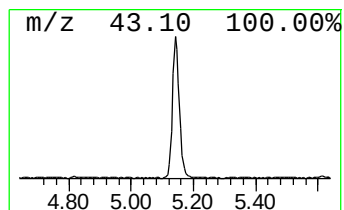
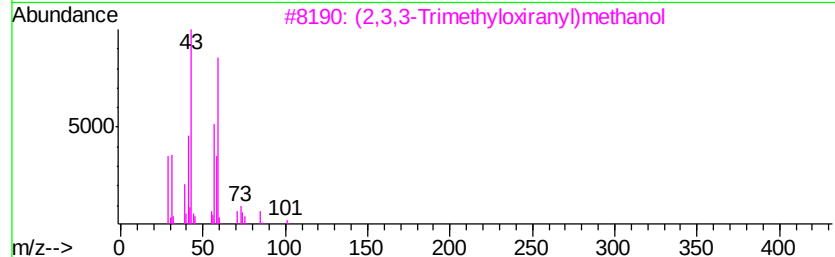
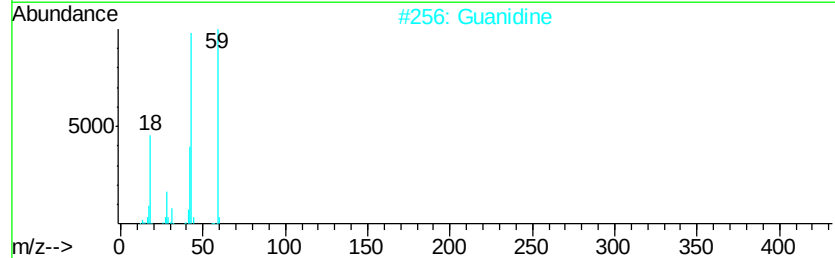
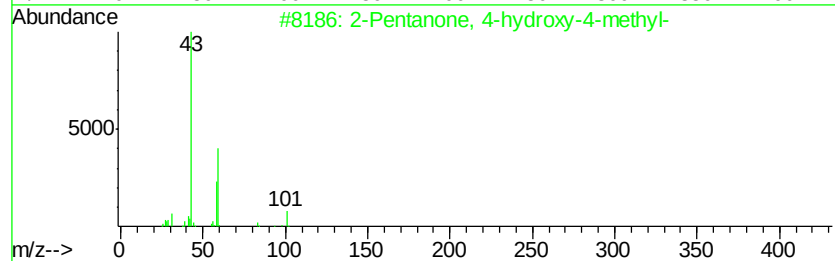
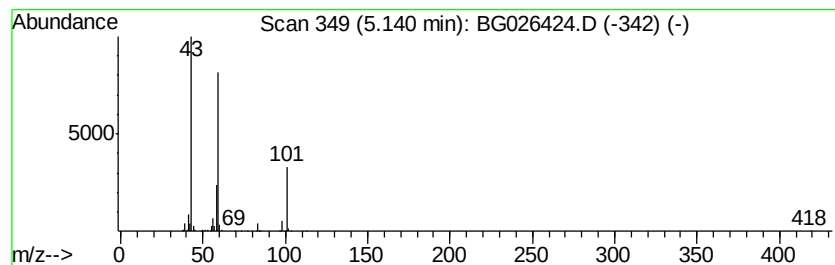
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG032017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	11.97 ng	449199	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	47
3		(2,3,3-Trimethyloxiran-yl)methanol	116	C6H12O2	1000306-64-7	38
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28
5		Acetone	58	C3H6O	000067-64-1	9



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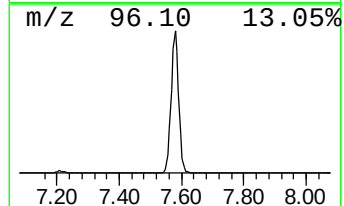
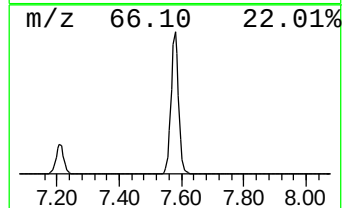
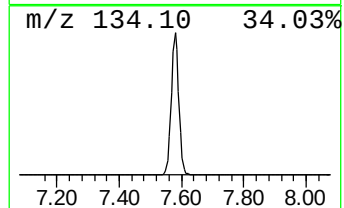
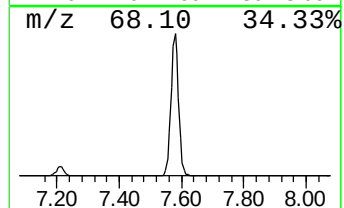
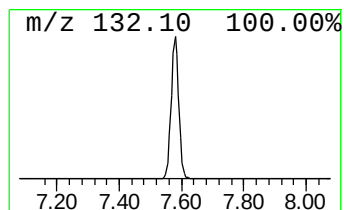
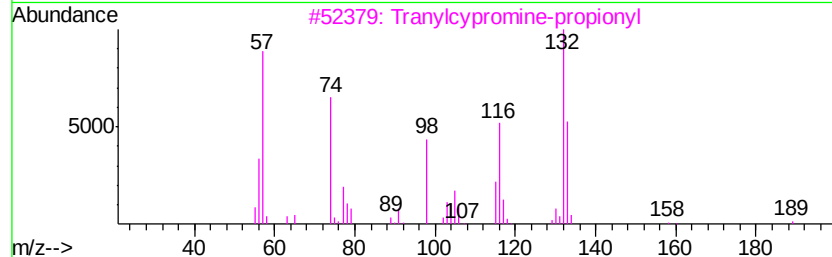
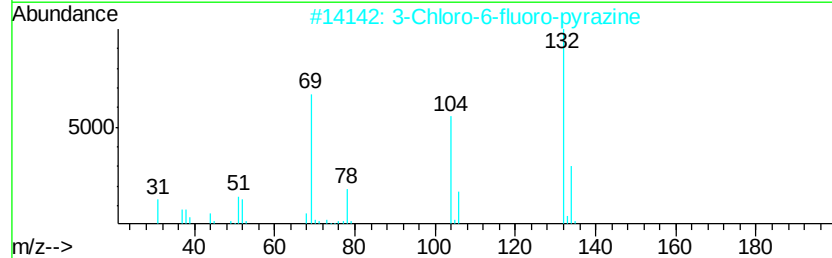
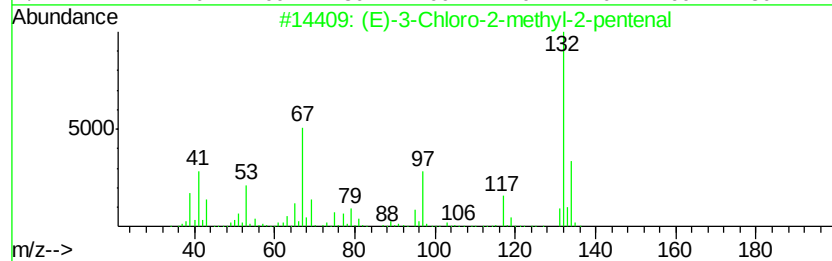
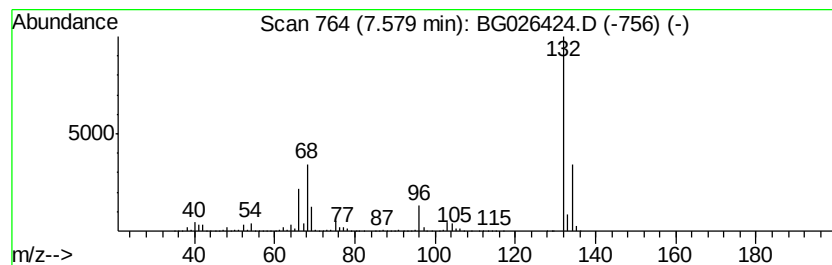
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Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	109.99 ng	4127020	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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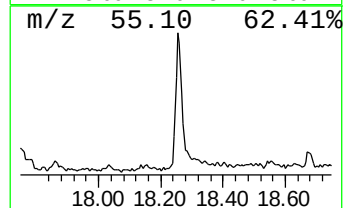
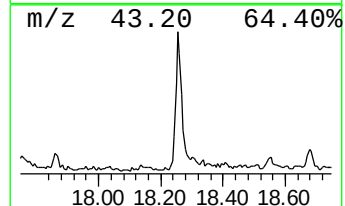
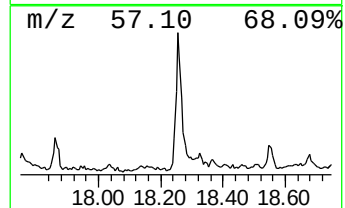
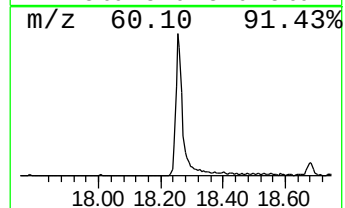
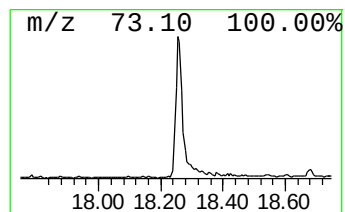
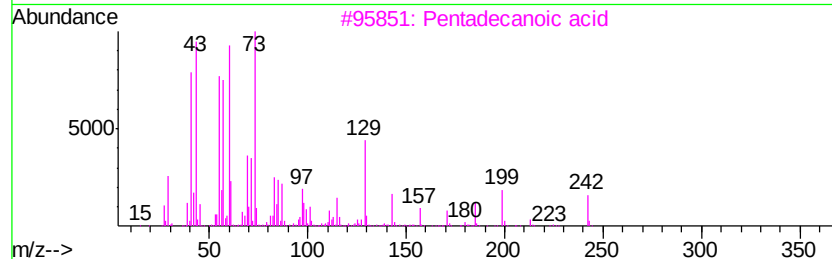
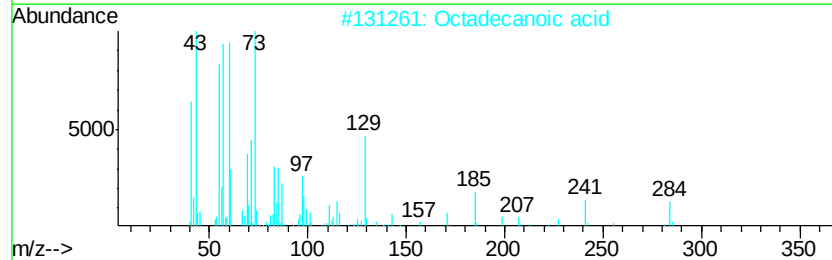
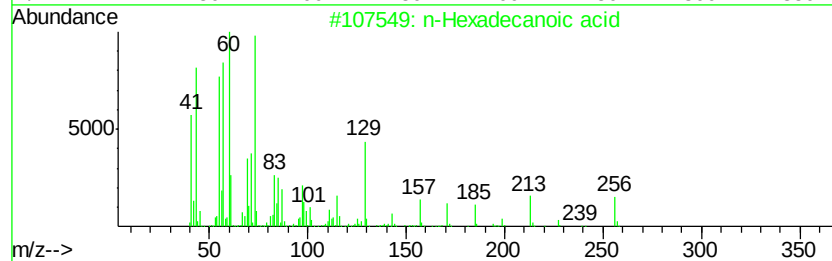
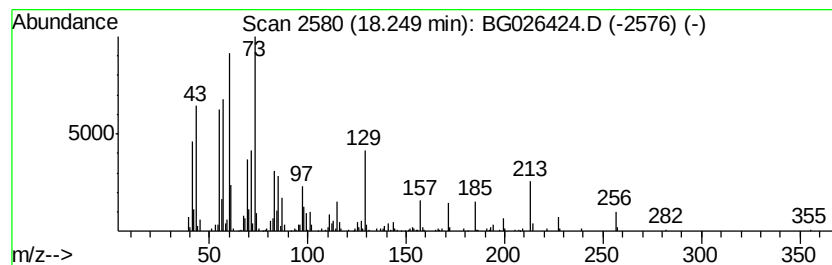
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TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.25	5.37 ng	532967	Phenanthrene-d10		17.38	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	89
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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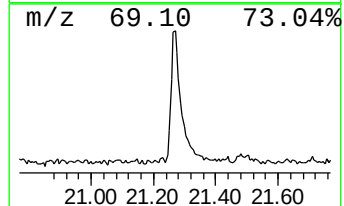
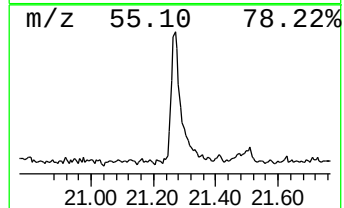
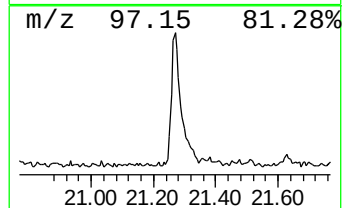
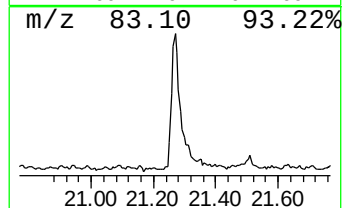
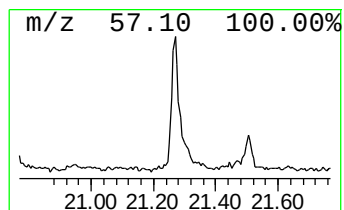
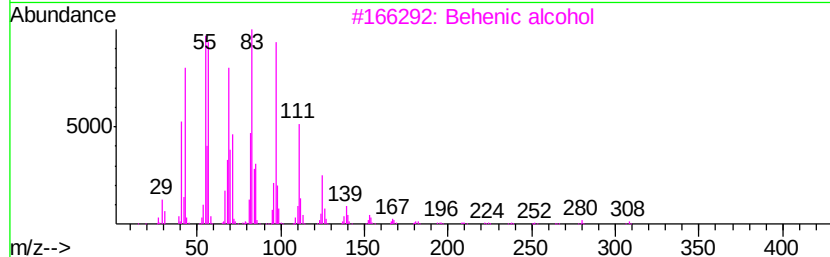
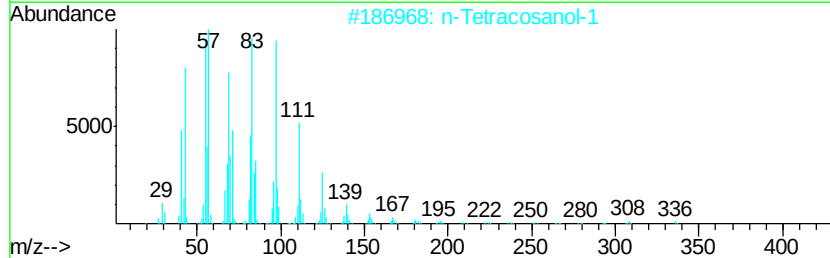
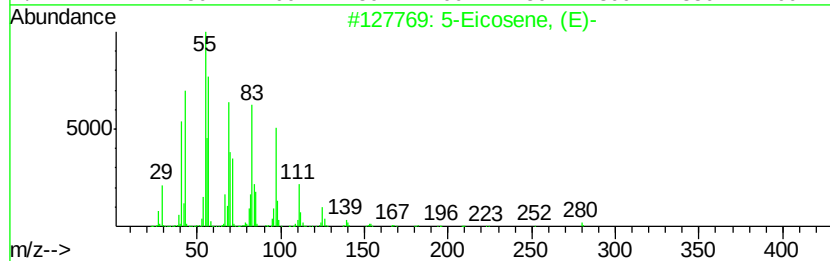
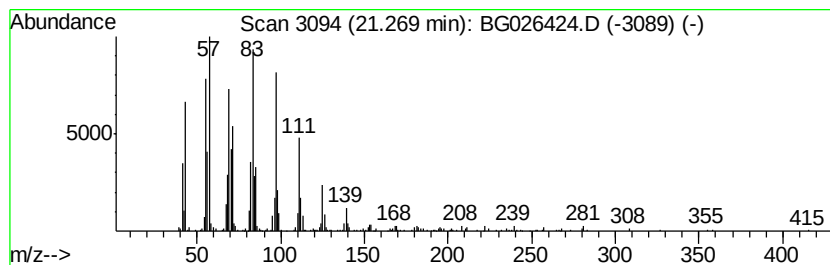
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	4.53 ng	600588	Chrysene-d12	21.63
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	5-Eicosene, (E)-	280 C20H40	074685-30-6	99
2	n-Tetracosanol-1	354 C24H50O	000506-51-4	95
3	Behenic alcohol	326 C22H46O	000661-19-8	95
4	9-Nonadecene	266 C19H38	031035-07-1	94
5	Pentafluoropropionic acid, tetra...	360 C17H29F5O2	006222-06-6	94



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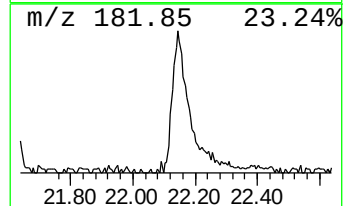
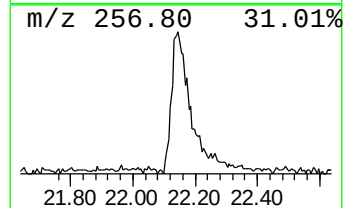
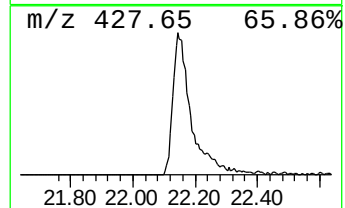
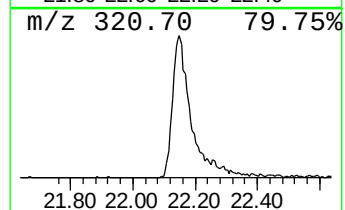
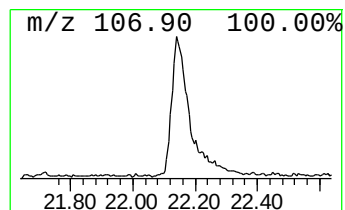
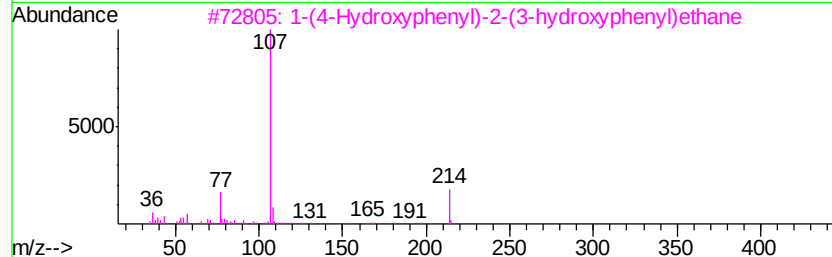
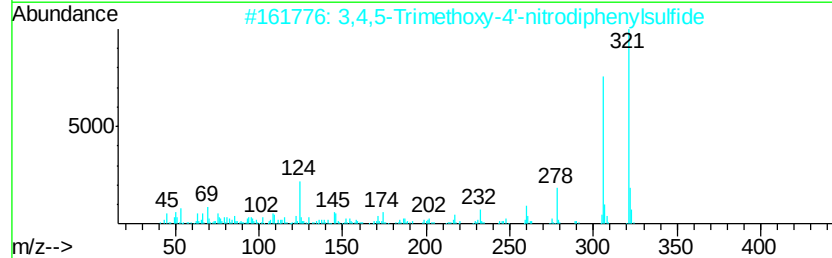
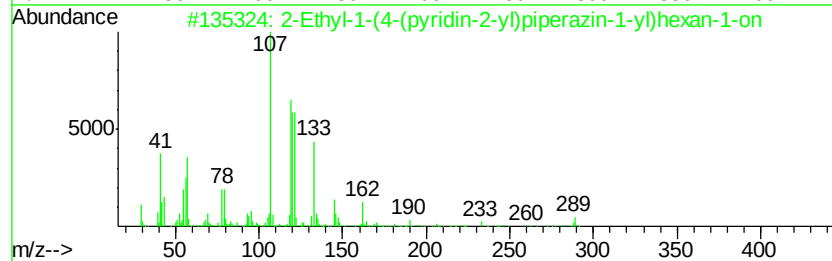
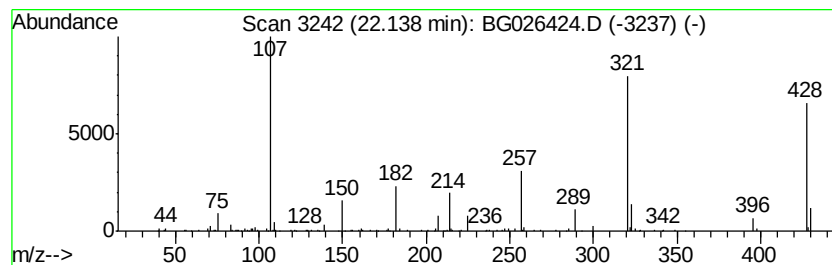
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown22.14 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.14	2.46 ng	325794	Chrysene-d12	21.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Ethyl-1-(4-(pyridin-2-yl)piper...	289	C17H27N3O	1000368-48-7	10
2		3,4,5-Trimethoxy-4'-nitrodipheny...	321	C15H15N05S	024891-42-7	10
3		1-(4-Hydroxyphenyl)-2-(3-hydroxy...	214	C14H14O2	037116-80-6	9
4		2-Methyl-2-bornene	150	C11H18	072540-93-3	9
5		4-Amino-5-nitro-6-[3,4,5-trimeth...	321	C13H15N5O5	1000254-14-1	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	12.0	ng	449199	1	8.04	750433	20.0
unknown7.58	7.58	110.0	ng	4127020	1	8.04	750433	20.0
n-Hexadecanoic acid	18.25	5.4	ng	532967	4	17.38	1985360	20.0
5-Eicosene, (E)-	21.27	4.5	ng	600588	5	21.63	2653620	20.0
unknown22.14	22.14	2.5	ng	325794	5	21.63	2653620	20.0