

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
 Data File : BF133248.D
 Acq On : 05 May 2023 00:12
 Operator : CG\JU
 Sample : 02598-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-241

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-BF042123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133248.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	477	482	490	rVB	250578	325332	7.07%	0.984%
2	5.339	548	553	556	rBV	4332067	4137604	89.86%	12.518%
3	6.363	722	727	730	rBV	3806929	4304736	93.49%	13.023%
4	6.722	785	788	792	rBV	1436166	1246771	27.08%	3.772%
5	7.292	880	885	888	rBV	2882193	2747706	59.68%	8.313%
6	8.010	1003	1007	1010	rBV	2149226	1669107	36.25%	5.050%
7	9.086	1186	1190	1193	rBV	5510236	4604256	100.00%	13.929%
8	9.757	1301	1304	1308	rBV	2053818	1821200	39.55%	5.510%
9	10.474	1422	1426	1429	rBV	385098	341486	7.42%	1.033%
10	10.545	1434	1438	1442	rBV	2829621	2655179	57.67%	8.033%
11	11.239	1552	1556	1559	rBV	2039947	1712441	37.19%	5.181%
12	11.263	1559	1560	1563	rVV	198422	111441	2.42%	0.337%
13	11.310	1563	1568	1573	rVB	42791	53545	1.16%	0.162%
14	11.780	1644	1648	1651	rBV2	315633	334403	7.26%	1.012%
15	12.451	1758	1762	1766	rBV	196515	196722	4.27%	0.595%
16	12.563	1777	1781	1785	rBV2	65048	78586	1.71%	0.238%
17	12.674	1794	1800	1803	rBV	168173	169150	3.67%	0.512%
18	12.827	1822	1826	1829	rBV	4069823	3557208	77.26%	10.762%
19	13.739	1977	1981	1995	rVB	152189	294581	6.40%	0.891%
20	13.874	1999	2004	2007	rBV	1103331	1144871	24.87%	3.464%
21	14.357	2083	2086	2089	rBV	55170	52449	1.14%	0.159%
22	14.727	2146	2149	2155	rVB4	37152	52447	1.14%	0.159%
23	14.886	2173	2176	2184	rVB	73488	143735	3.12%	0.435%
24	14.974	2188	2191	2196	rVV4	47061	65320	1.42%	0.198%
25	15.227	2231	2234	2239	rBV	48187	57850	1.26%	0.175%
26	15.292	2240	2245	2249	rBV	947038	1102965	23.96%	3.337%
27	15.745	2318	2322	2328	rBV3	38950	73127	1.59%	0.221%

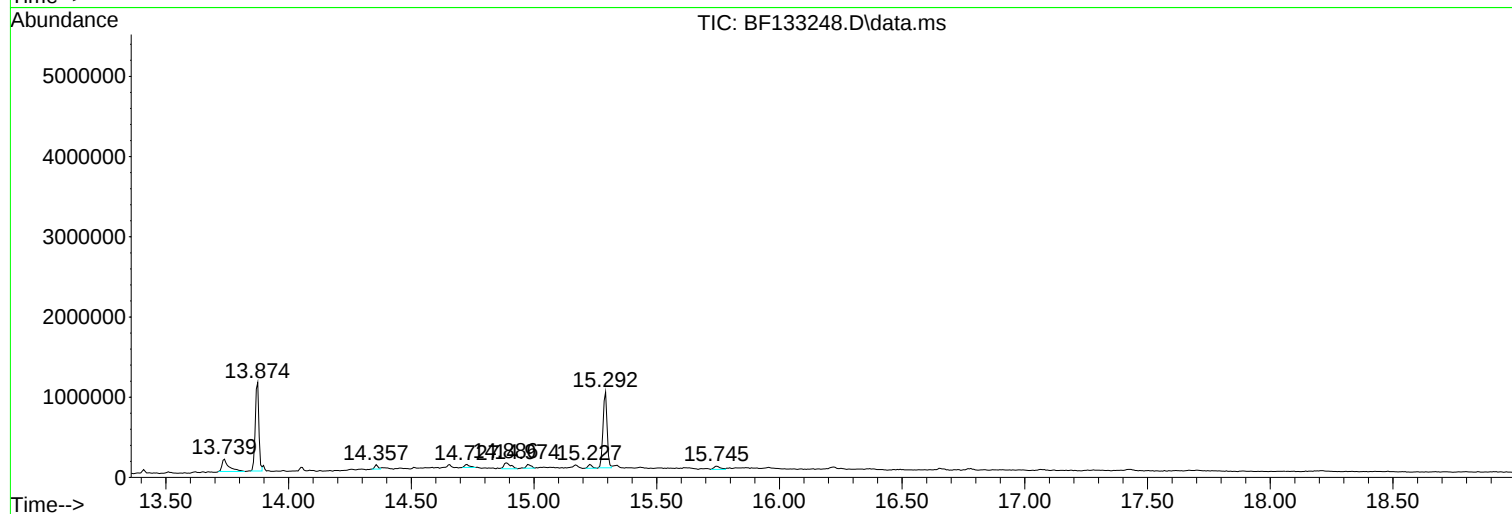
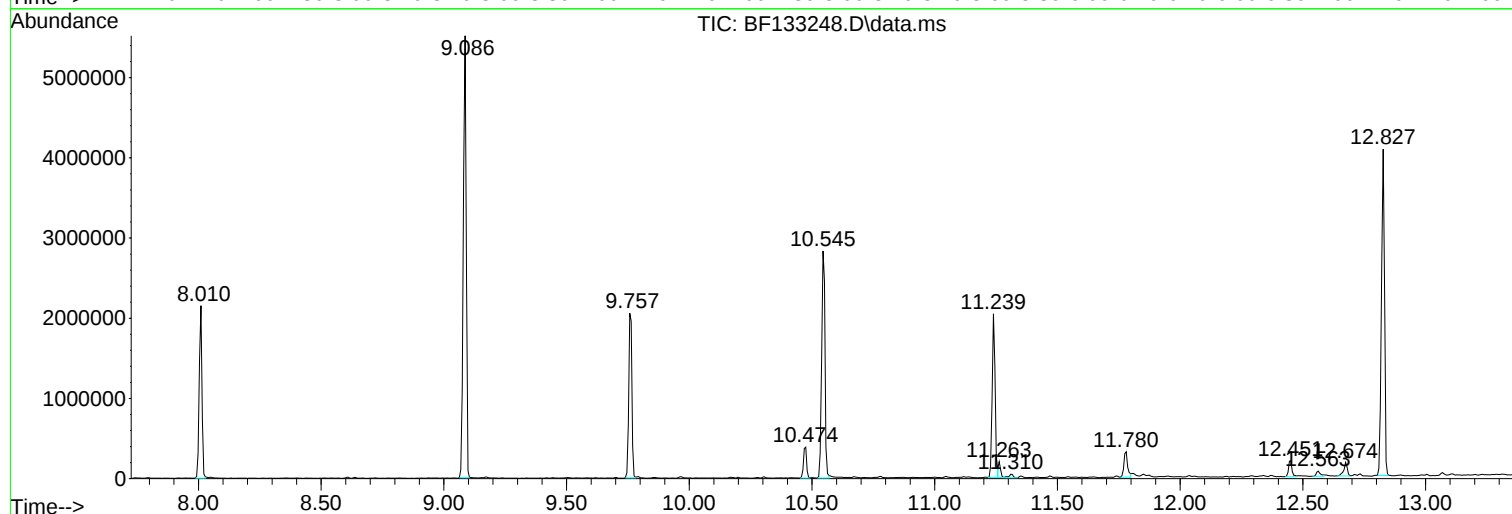
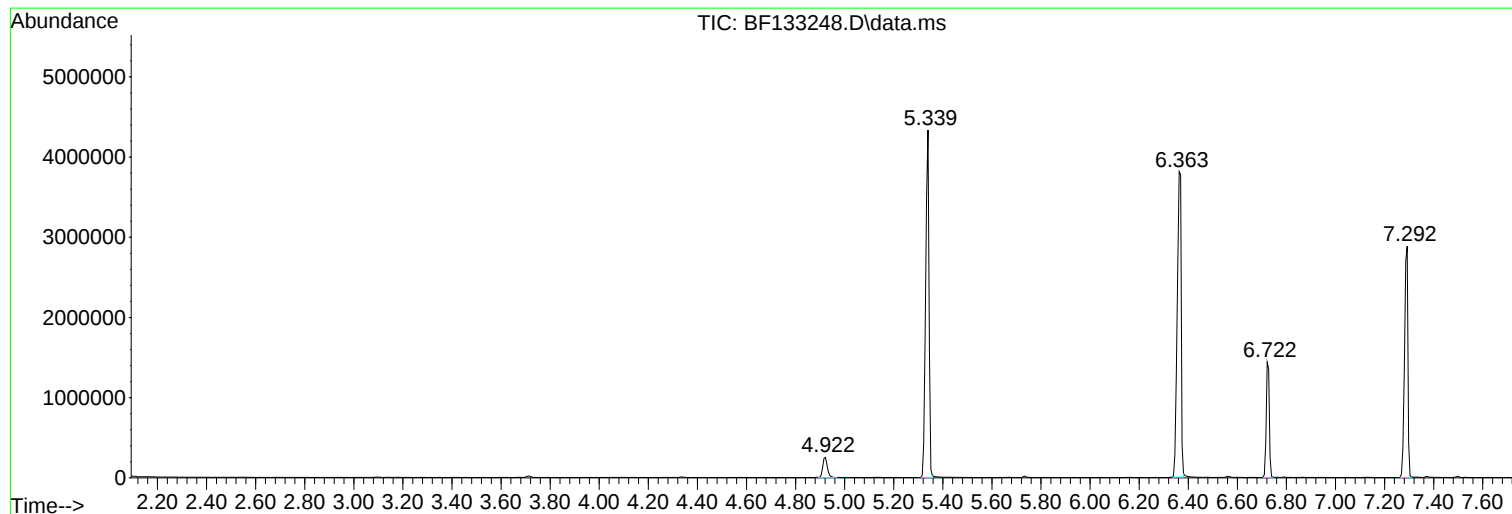
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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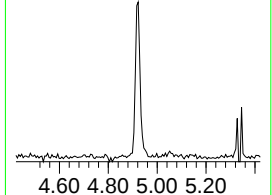
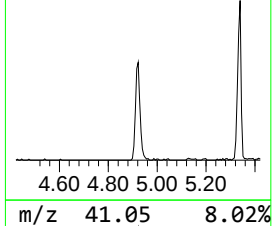
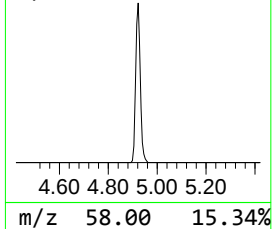
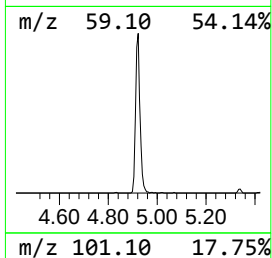
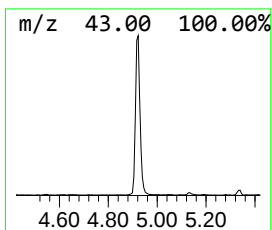
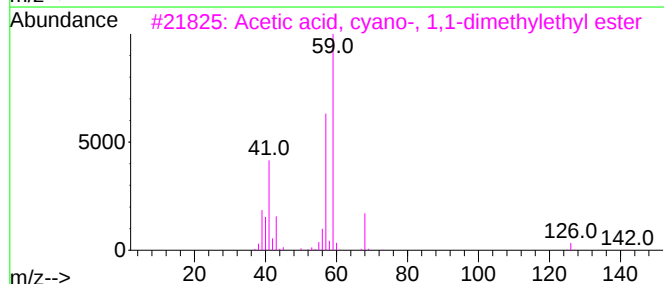
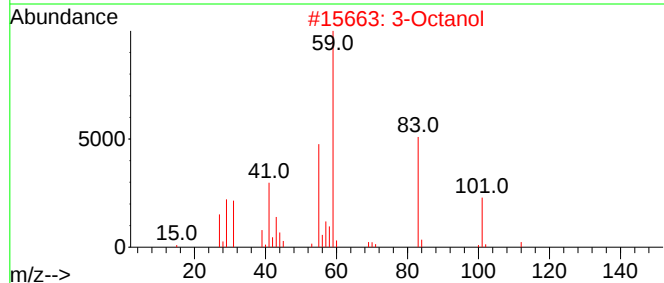
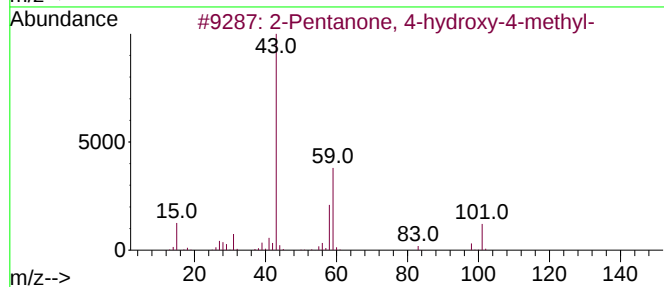
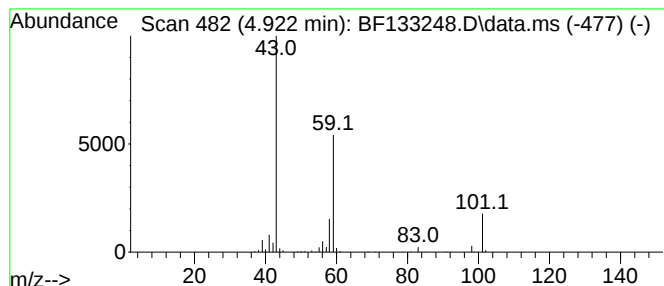
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	5.22 ng	325332	1,4-Dichlorobenzene-d4	6.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		



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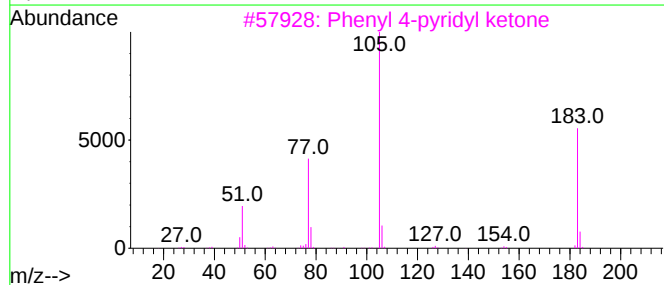
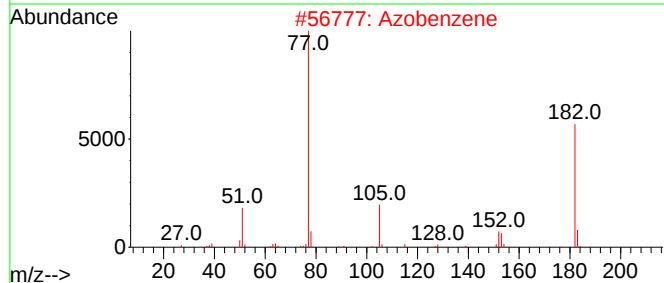
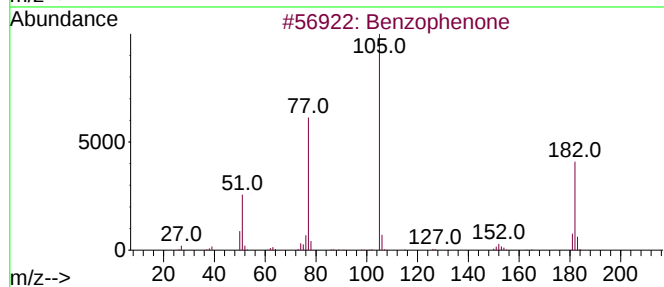
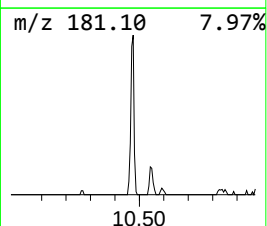
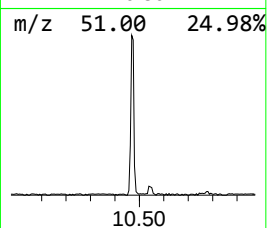
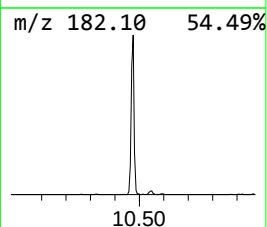
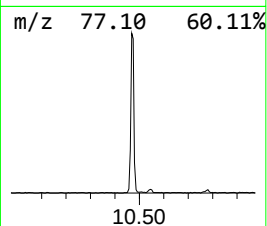
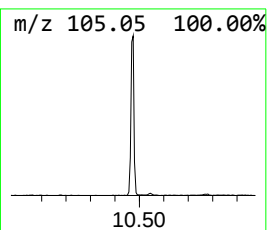
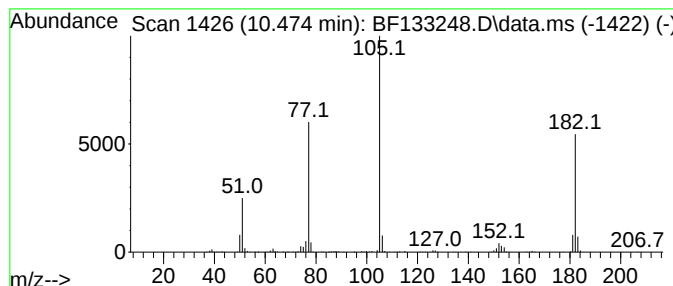
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.75 ng	341486	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47



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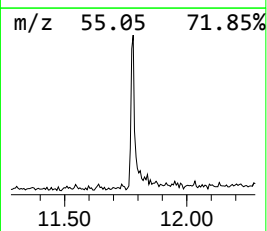
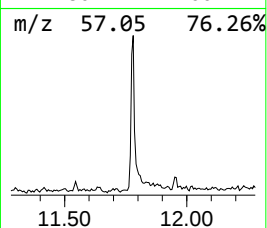
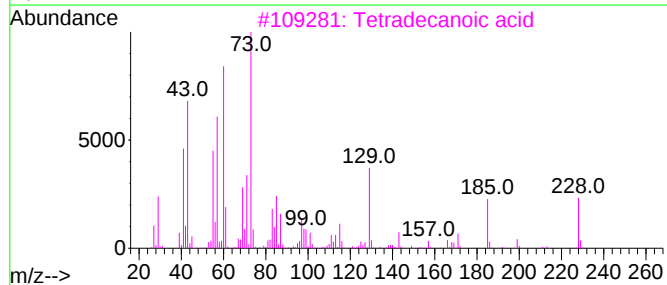
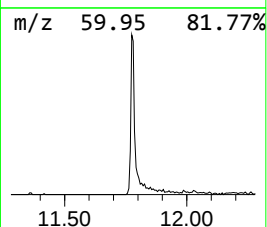
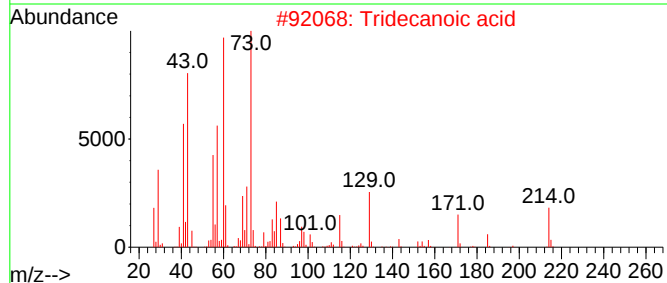
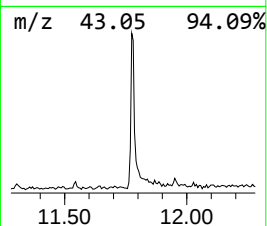
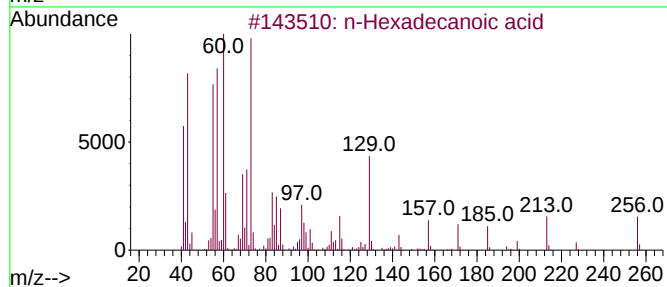
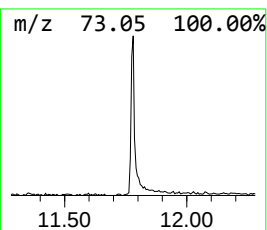
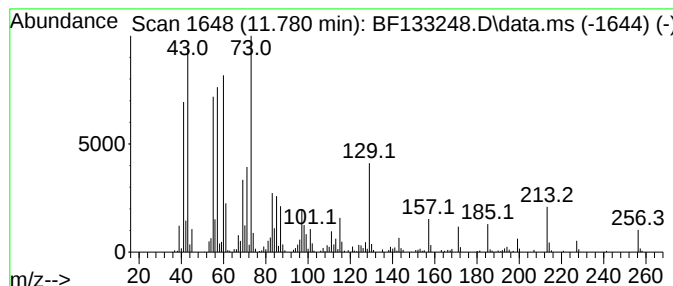
Instrument :
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ClientSampleId :
VNJ-241

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.780	3.91 ng	334403	Phenanthrene-d10		11.239	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
5	n-Decanoic acid		172	C10H20O2	000334-48-5	68



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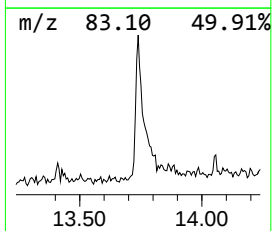
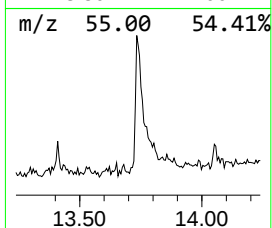
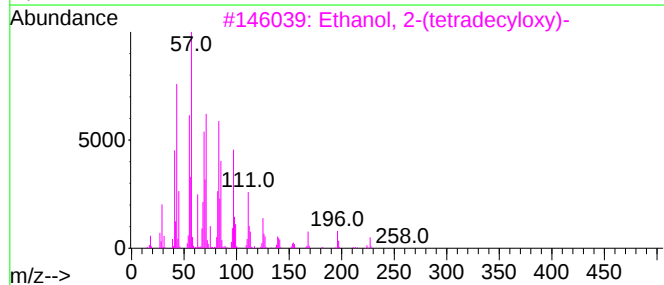
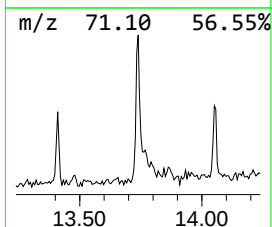
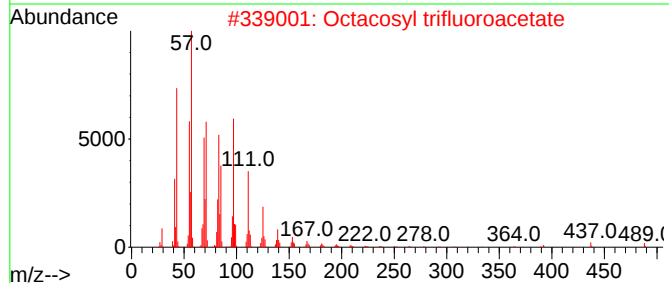
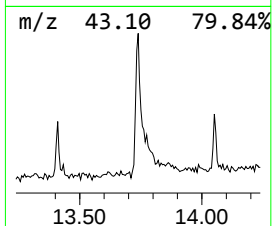
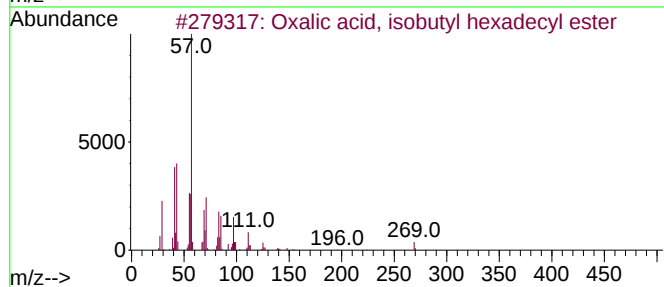
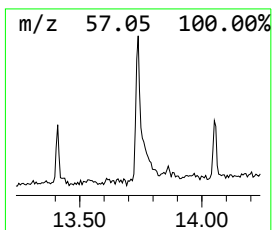
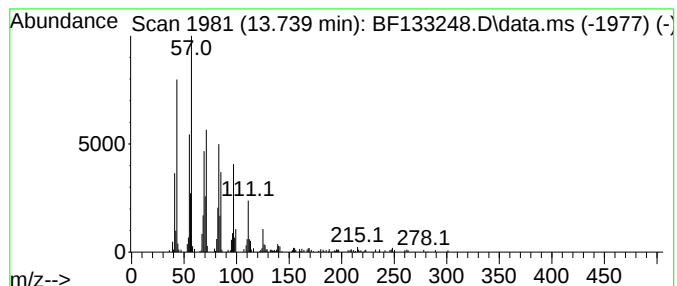
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Peak Number 5 Oxalic acid, isobutyl hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	5.15 ng	294581	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
5			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	90



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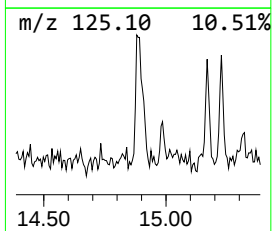
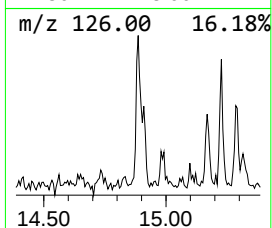
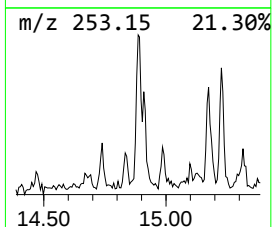
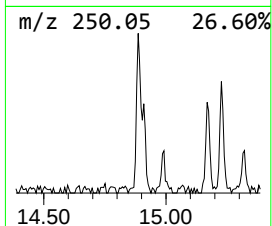
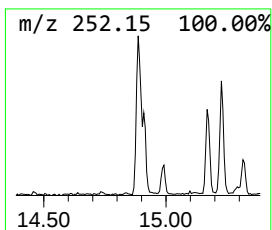
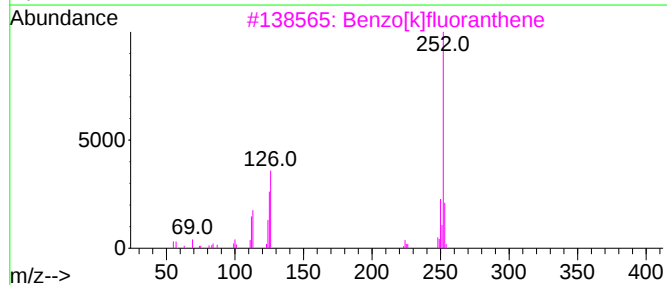
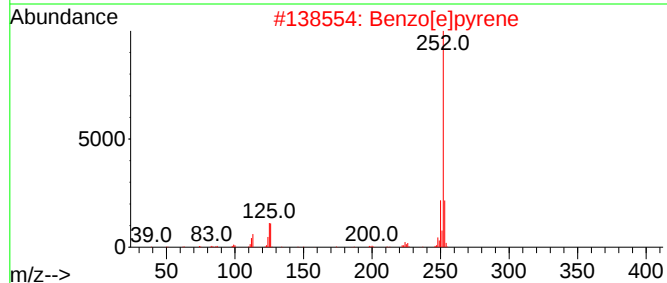
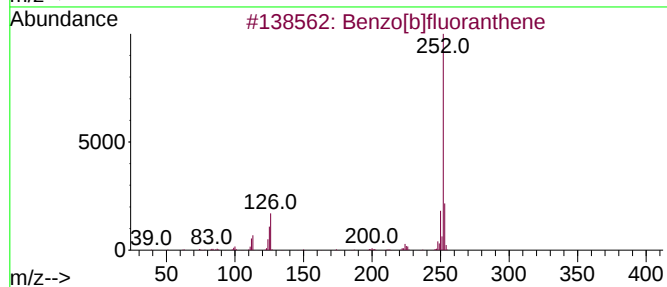
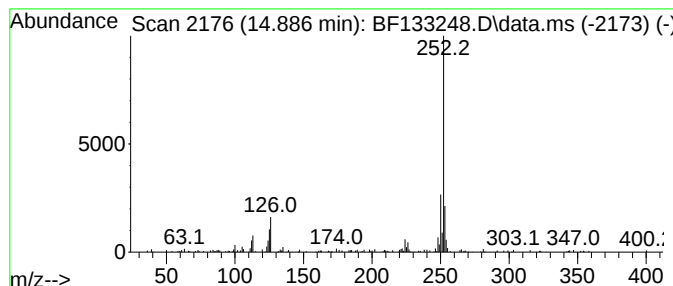
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	2.61 ng	143735	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	97
2			Benzo[e]pyrene	252	C20H12	000192-97-2	95
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Perylene	252	C20H12	000198-55-0	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.922	5.2	ng	325332	1	6.728	1246770	20.0
Benzophenone	10.475	3.8	ng	341486	3	9.757	1821200	20.0
n-Hexadecanoic ...	11.780	3.9	ng	334403	4	11.239	1712440	20.0
Oxalic acid, is...	13.739	5.2	ng	294581	5	13.874	1144870	20.0
Benzo[e]pyrene	14.886	2.6	ng	143735	6	15.292	1102970	20.0