

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071423\
 Data File : BF134282.D
 Acq On : 14 Jul 2023 10:16
 Operator : CG\JU
 Sample : PB154160BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB154160BL

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134282.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.475	401	406	422	rBV	693014	775807	20.91%	3.313%
2	5.093	505	511	523	rBV	1224840	1879404	50.66%	8.025%
3	5.487	573	578	581	rBV	2586719	2486161	67.01%	10.616%
4	5.869	639	643	647	rBV	43295	38847	1.05%	0.166%
5	6.487	743	748	751	rBV	2432063	2490122	67.12%	10.633%
6	6.840	805	808	826	rBV	576843	519264	14.00%	2.217%
7	7.410	900	905	908	rBV	1779303	1632920	44.01%	6.973%
8	8.122	1022	1026	1038	rBV	860391	685404	18.47%	2.927%
9	9.204	1205	1210	1213	rBV	3653052	3157386	85.10%	13.482%
10	9.881	1321	1325	1329	rBV	962792	781495	21.06%	3.337%
11	10.680	1456	1461	1464	rBV	2382884	2291614	61.77%	9.785%
12	11.375	1575	1579	1587	rBV	970774	879789	23.71%	3.757%
13	12.980	1847	1852	1855	rBV	4025843	3710004	100.00%	15.842%
14	14.039	2028	2032	2041	rBV	881773	820903	22.13%	3.505%
15	14.821	2161	2165	2172	rBV2	37703	46643	1.26%	0.199%
16	15.168	2221	2224	2228	rBV	44061	54277	1.46%	0.232%
17	15.551	2283	2289	2298	rBV	607971	905093	24.40%	3.865%
18	16.027	2365	2370	2380	rVB	59817	106456	2.87%	0.455%
19	16.562	2456	2461	2468	rBV4	50647	97889	2.64%	0.418%
20	17.198	2565	2569	2576	rVB2	30867	59197	1.60%	0.253%

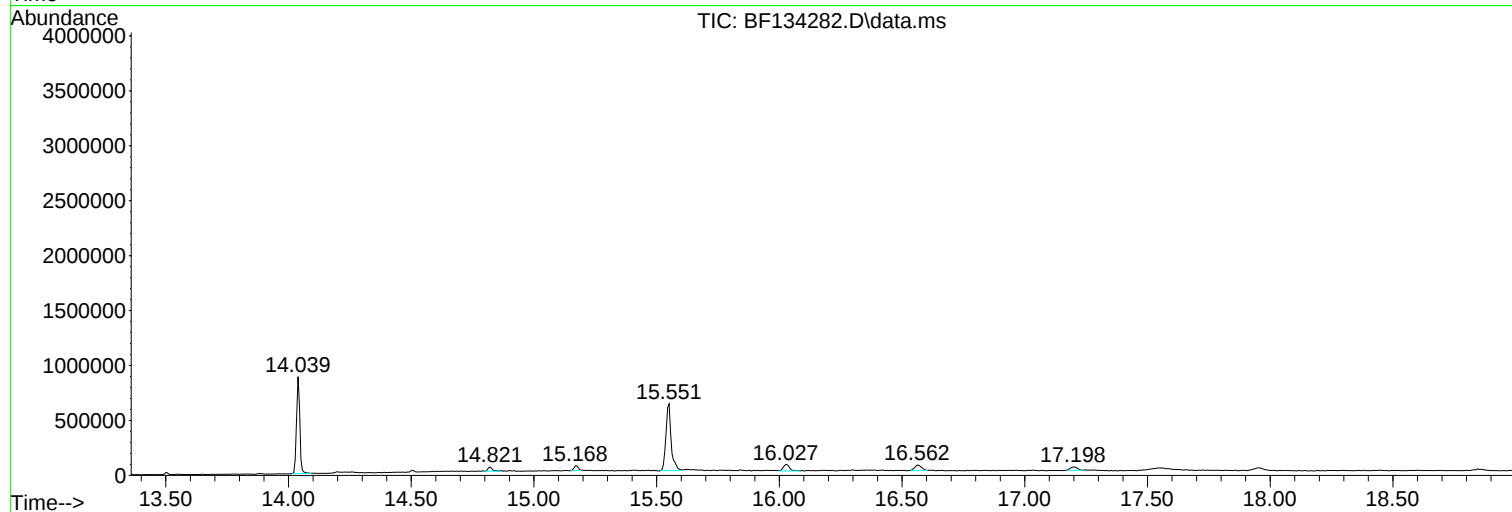
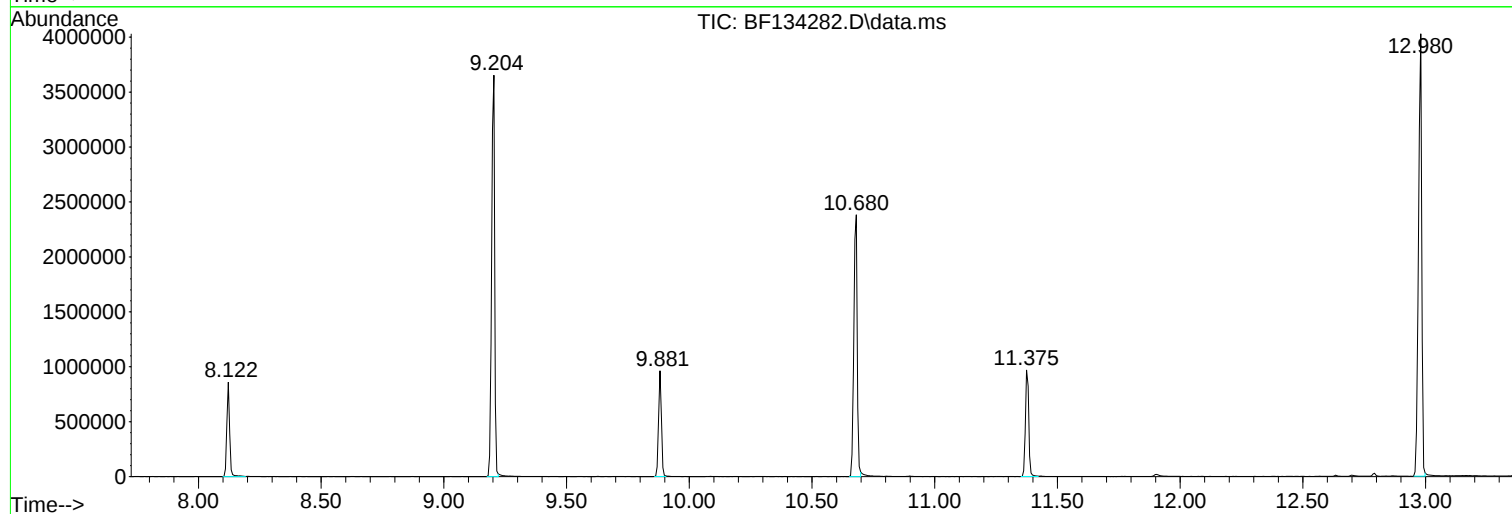
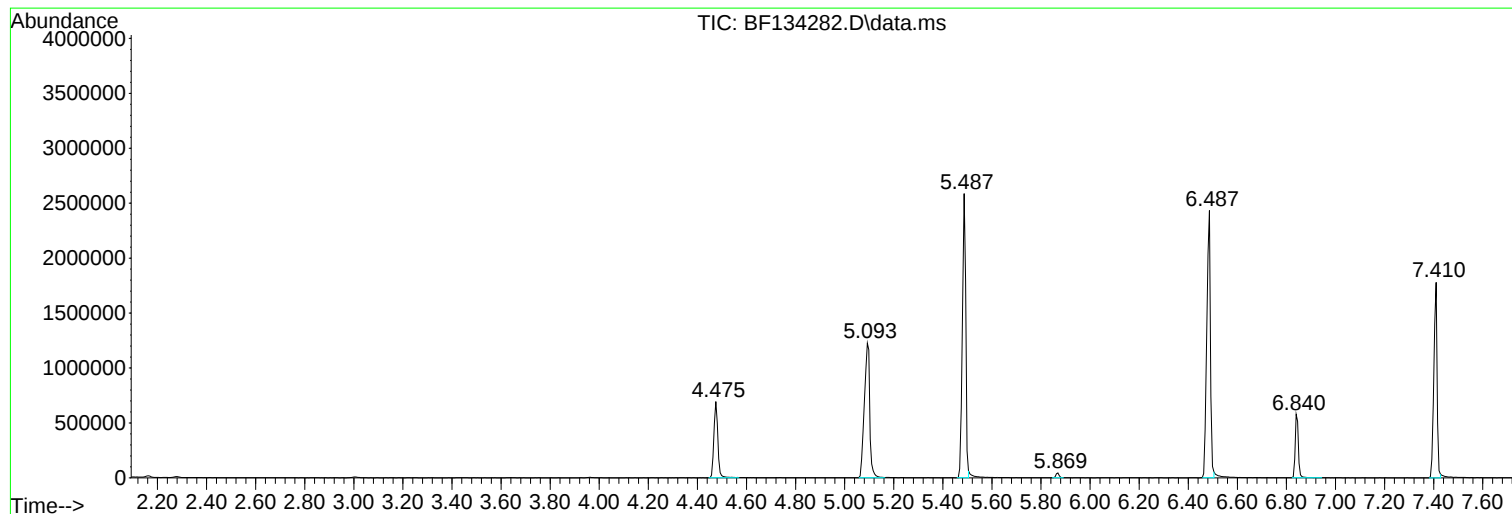
Sum of corrected areas: 23418675

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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Instrument :
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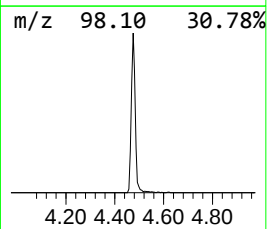
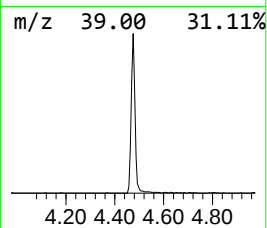
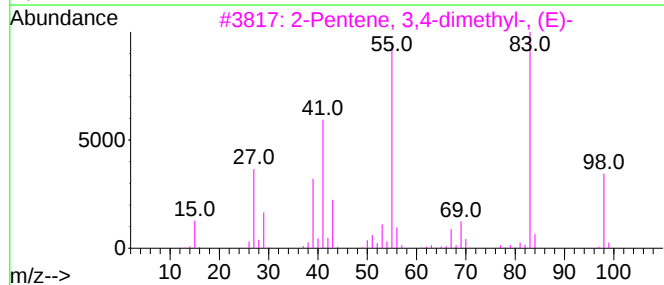
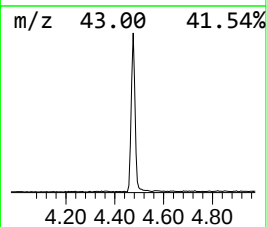
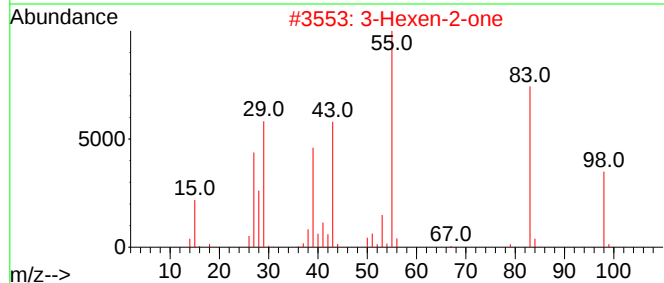
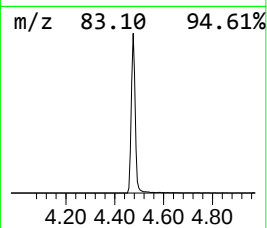
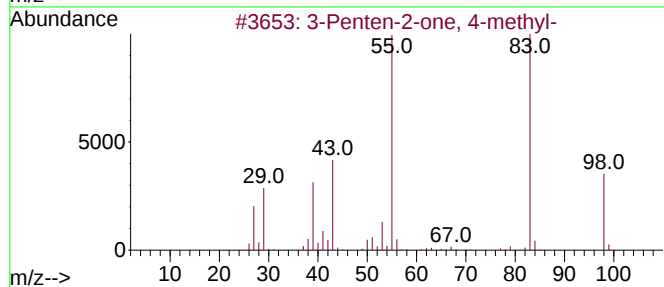
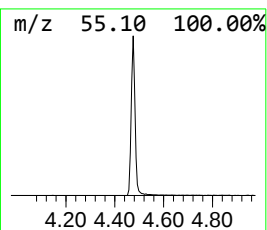
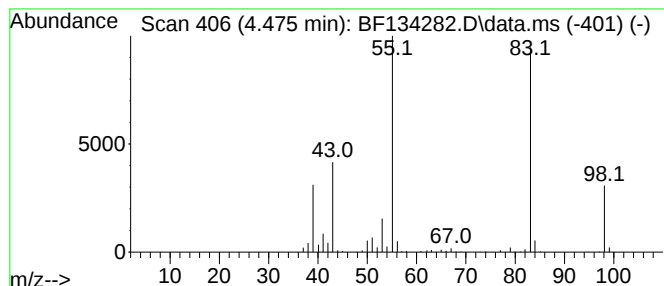
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.475	29.88 ng	775807	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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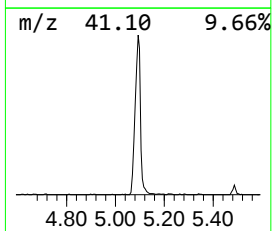
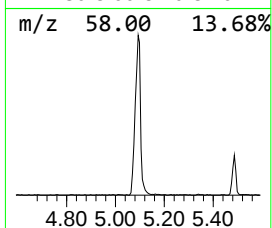
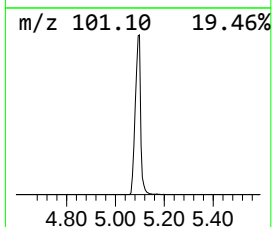
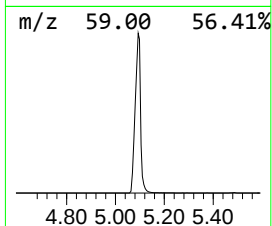
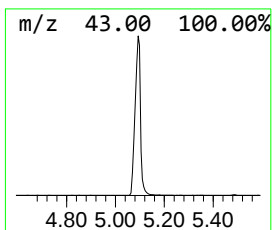
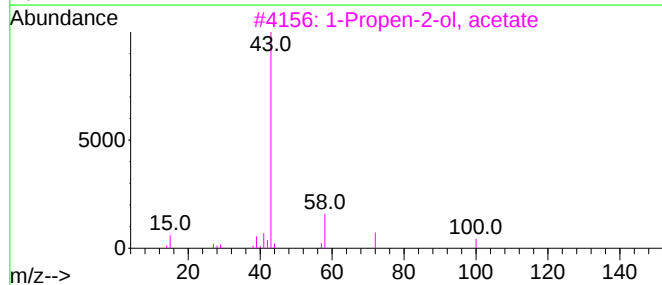
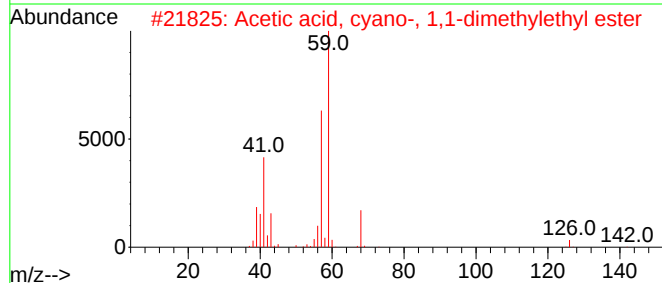
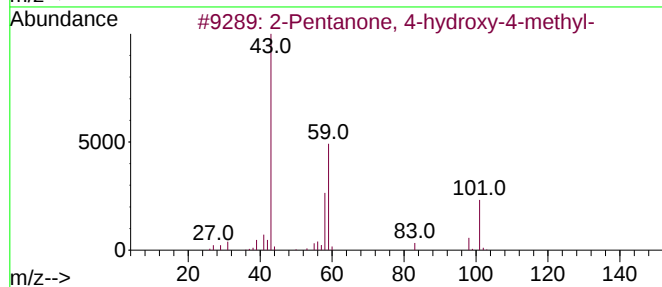
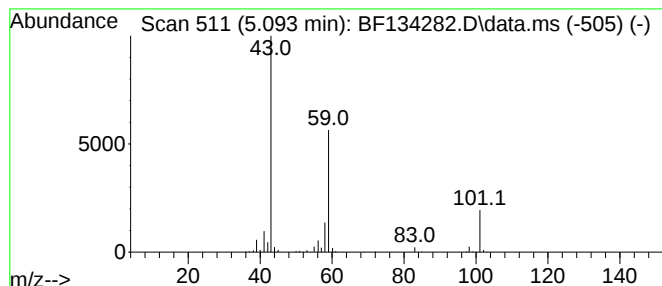
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.093	72.39 ng	1879400	1,4-Dichlorobenzene-d4	6.840	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
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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ALS Vial : 3 Sample Multiplier: 1

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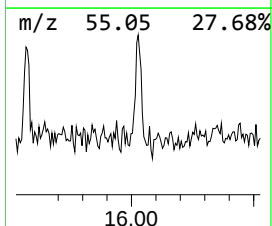
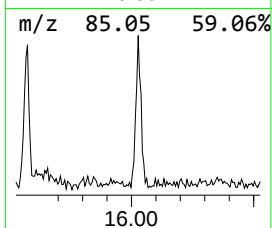
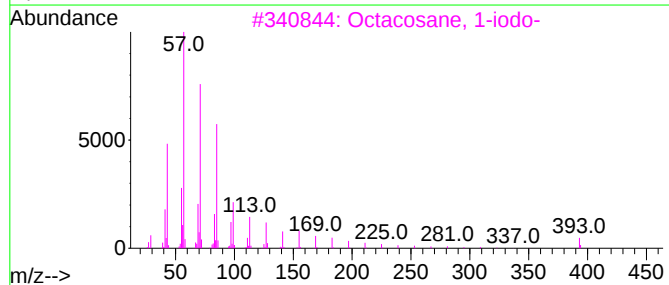
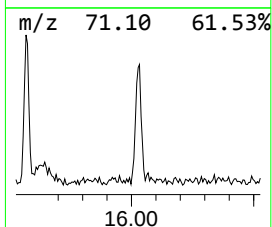
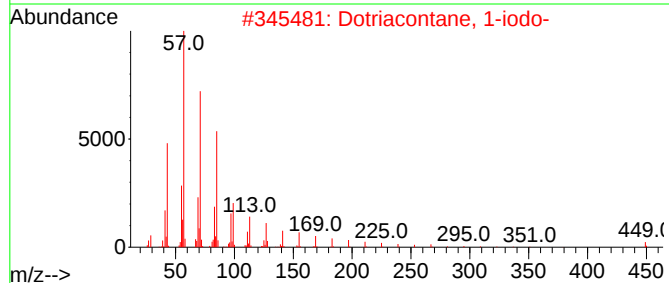
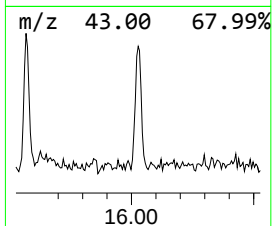
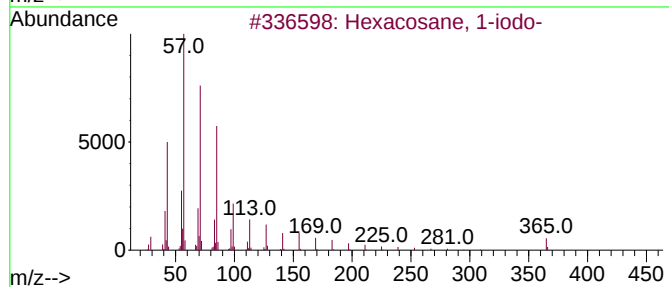
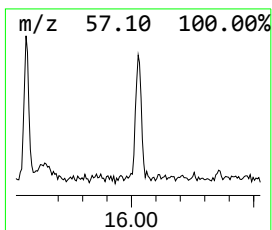
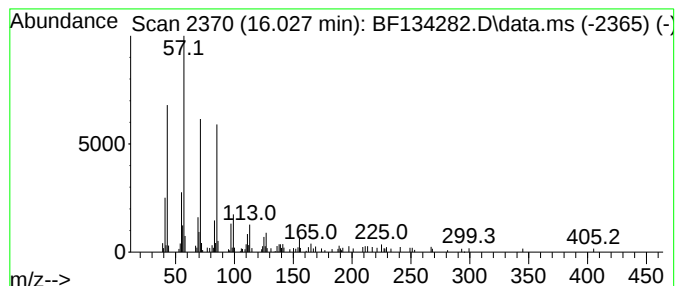
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexacosane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	2.35 ng	106456	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	87
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
3			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	87
4			Docosane	310	C22H46	000629-97-0	86
5			Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	86



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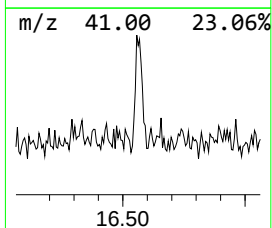
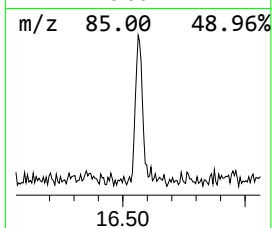
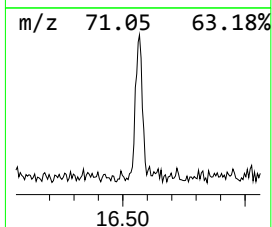
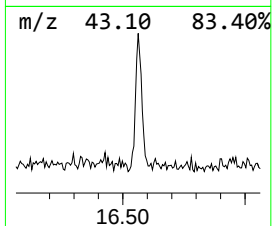
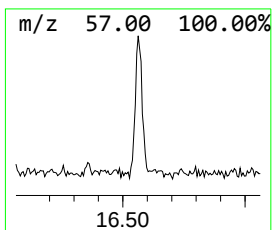
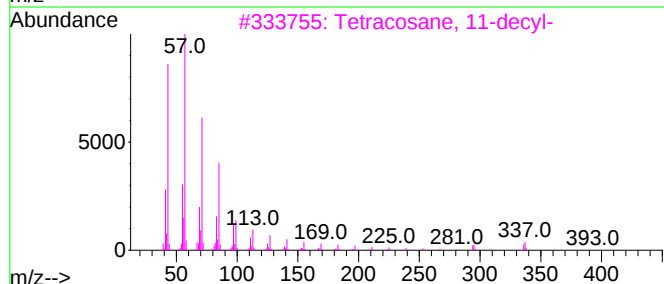
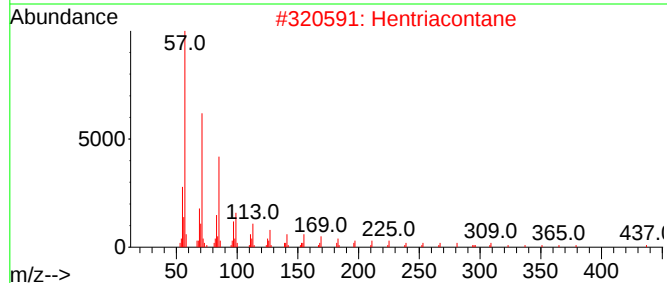
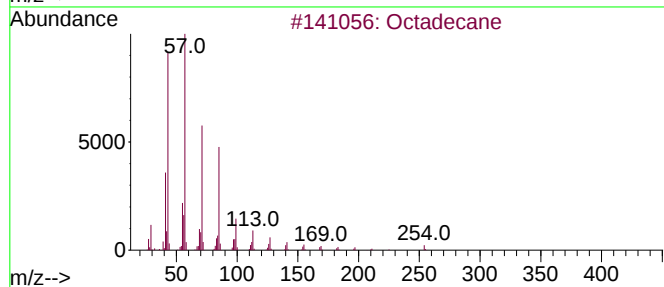
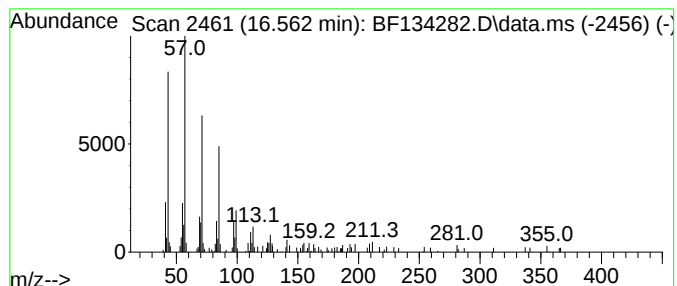
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Peak Number 4 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.563	2.16 ng	97889	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	94
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Hexacosane, 9-octyl-	479	C34H70	055429-83-9	90



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.475	29.9	ng	775807	1	6.840	519264	20.0
2-Pentanone, 4-...	5.093	72.4	ng	1879400	1	6.840	519264	20.0
Hexacosane, 1-i...	16.027	2.4	ng	106456	6	15.551	905093	20.0
Octadecane	16.563	2.2	ng	97889	6	15.551	905093	20.0