

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
 Data File : BF136487.D
 Acq On : 11 Dec 2023 13:23
 Operator : CG\JU
 Sample : PB157455BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB157455BL

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-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136487.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.463	394	404	407	rBV	3600534	5823591	100.00%	14.437%
2	4.704	441	445	449	rBV	81419	82988	1.43%	0.206%
3	5.069	497	507	510	rBV	2138002	3757059	64.51%	9.314%
4	5.457	567	573	576	rBV	3508991	3748546	64.37%	9.293%
5	5.822	632	635	639	rBV	369875	327358	5.62%	0.812%
6	6.446	733	741	744	rBV	3230243	3882045	66.66%	9.624%
7	6.793	797	800	804	rBV	958273	778209	13.36%	1.929%
8	7.357	890	896	899	rBV	2123327	2404181	41.28%	5.960%
9	8.069	1012	1017	1021	rBV	1159147	1085509	18.64%	2.691%
10	9.151	1195	1201	1204	rBV	4862838	4928364	84.63%	12.218%
11	9.828	1310	1316	1319	rBV	1605757	1307731	22.46%	3.242%
12	10.628	1445	1452	1455	rBV	3084620	3170360	54.44%	7.860%
13	11.322	1565	1570	1573	rBV	1689033	1406376	24.15%	3.487%
14	12.922	1837	1842	1845	rBV	5271684	5305077	91.10%	13.152%
15	13.974	2017	2021	2024	rBV	1146721	1031652	17.72%	2.558%
16	15.274	2238	2242	2250	rVB3	40648	61542	1.06%	0.153%
17	15.451	2266	2272	2277	rBV	608607	740213	12.71%	1.835%
18	15.498	2277	2280	2286	rVB	56841	75895	1.30%	0.188%
19	15.786	2324	2329	2336	rBV2	37162	69901	1.20%	0.173%
20	15.951	2352	2357	2362	rVB2	47440	73303	1.26%	0.182%
21	16.398	2427	2433	2441	rBV5	31303	70352	1.21%	0.174%
22	16.480	2441	2447	2455	rVB2	41478	79322	1.36%	0.197%
23	17.104	2546	2553	2557	rBV4	27368	60898	1.05%	0.151%
24	17.839	2671	2678	2686	rVB6	25310	66317	1.14%	0.164%

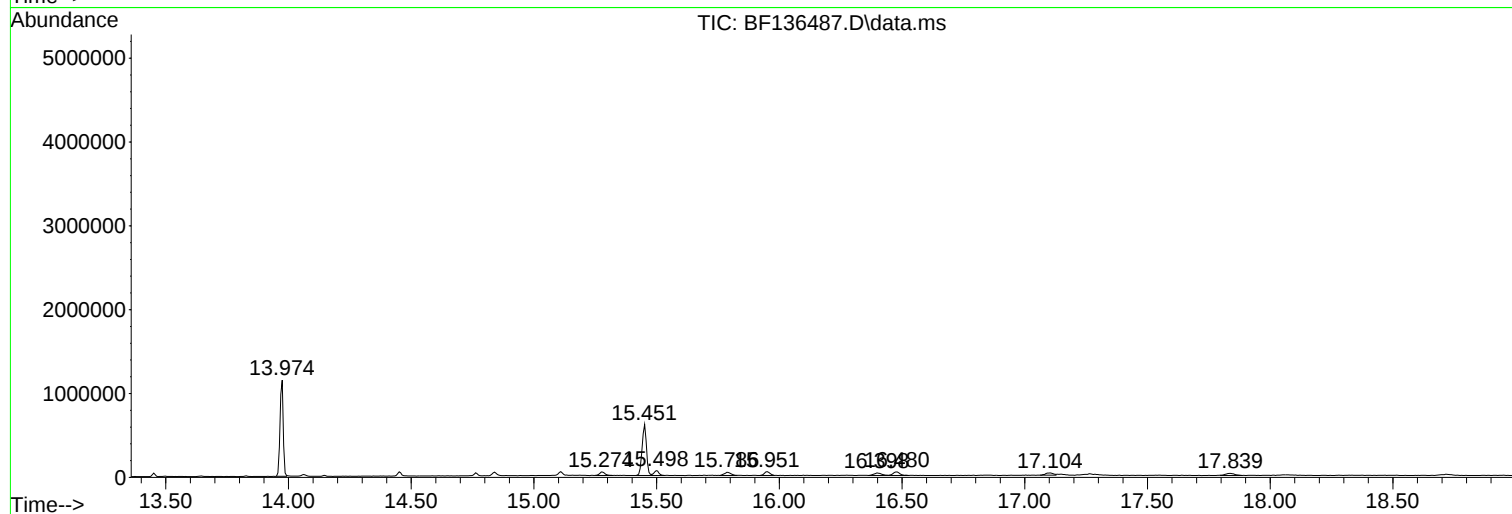
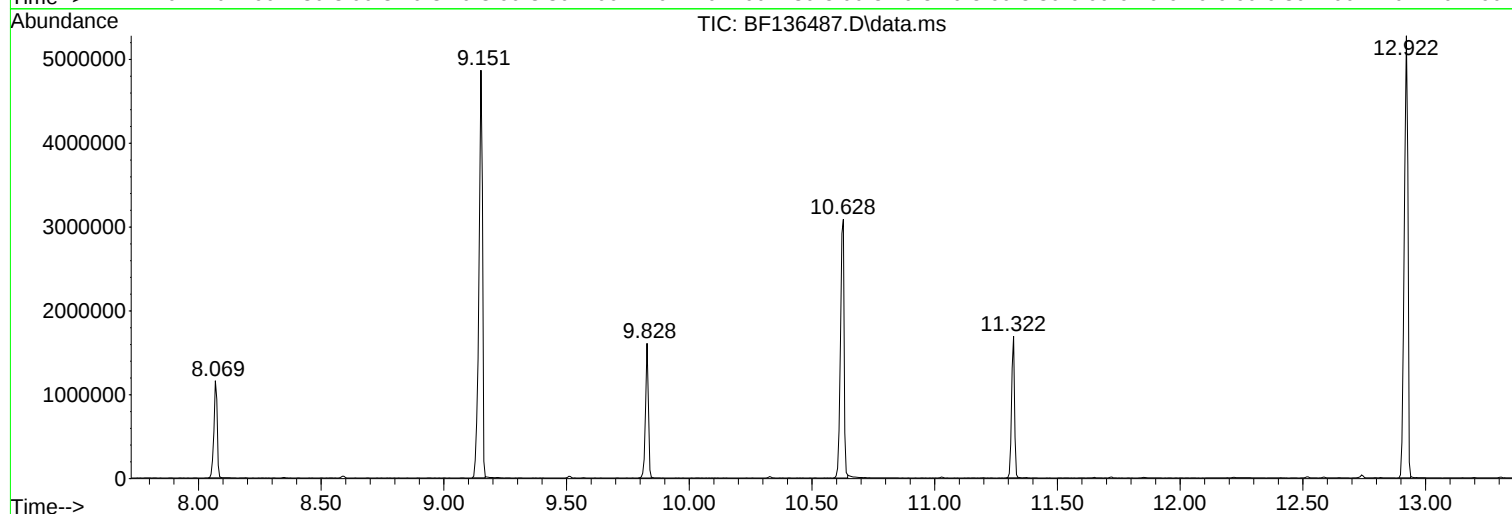
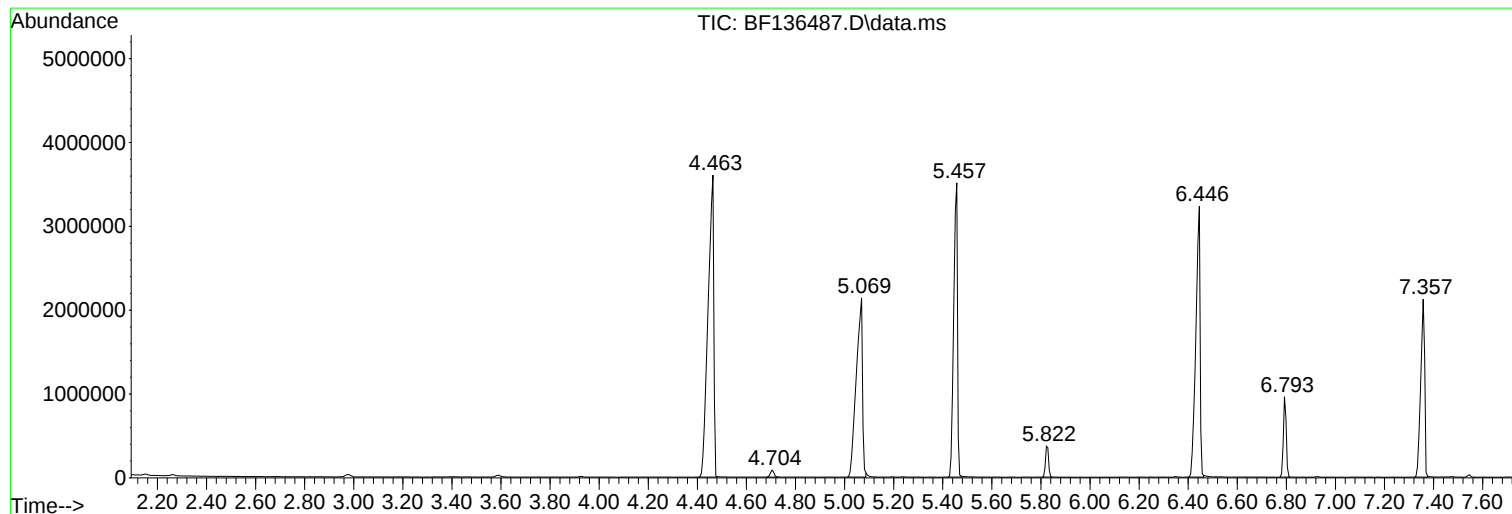
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ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB157455BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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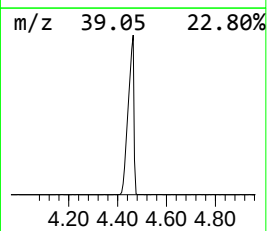
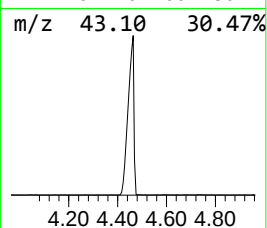
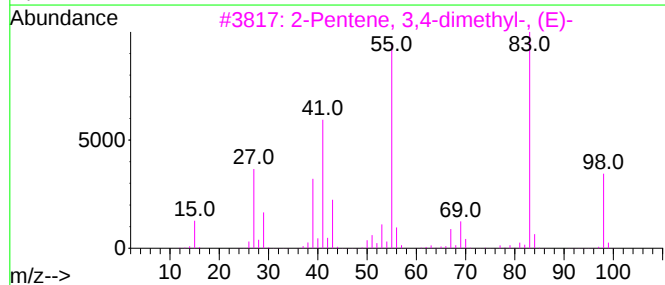
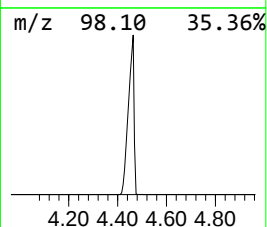
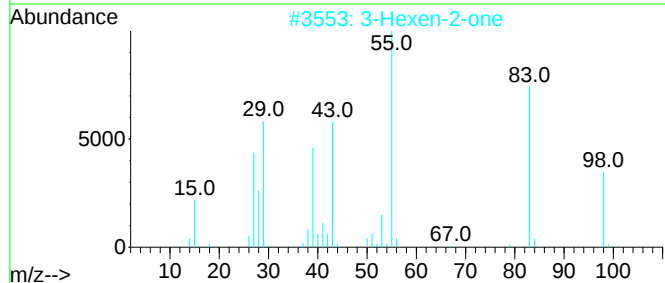
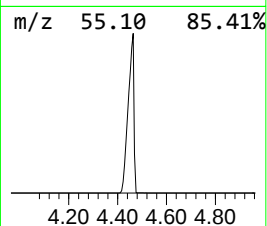
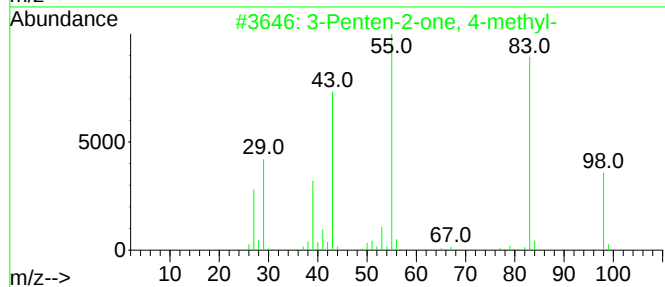
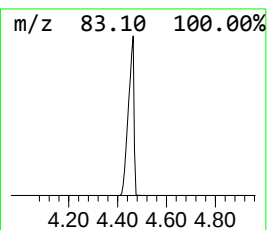
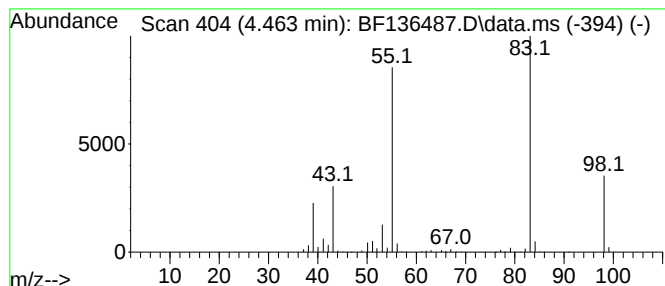
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.463	149.67 ng	5823590	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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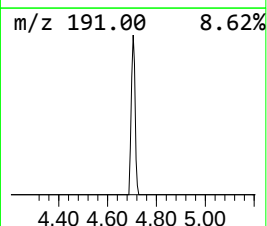
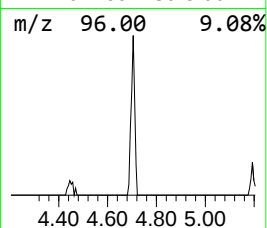
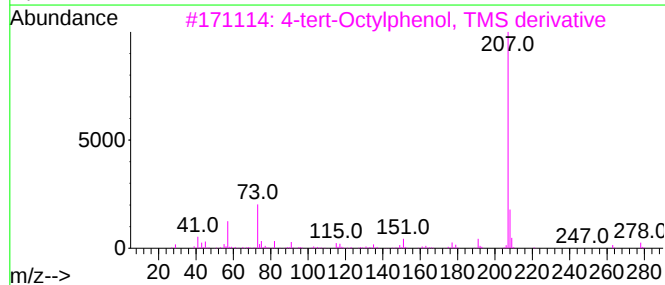
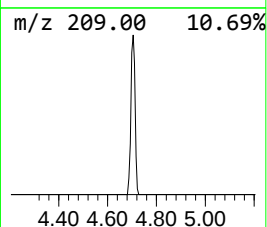
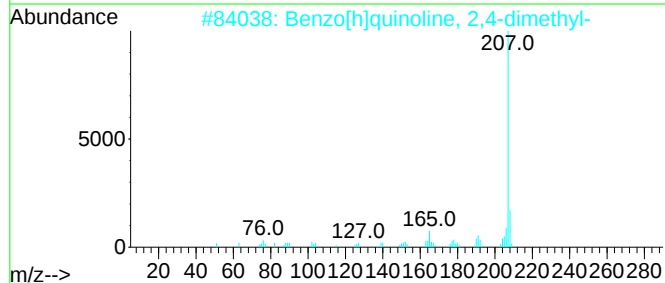
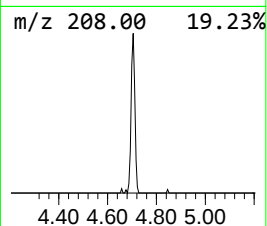
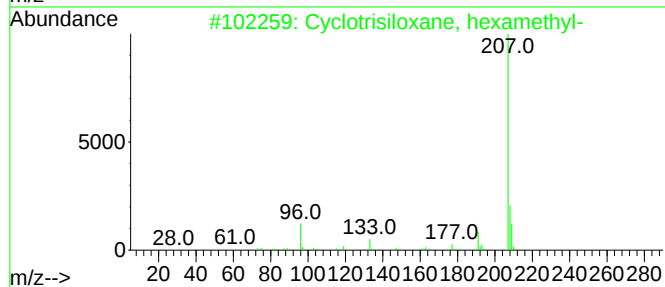
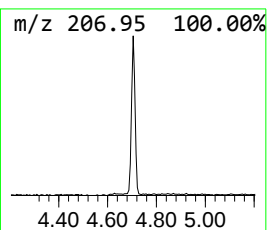
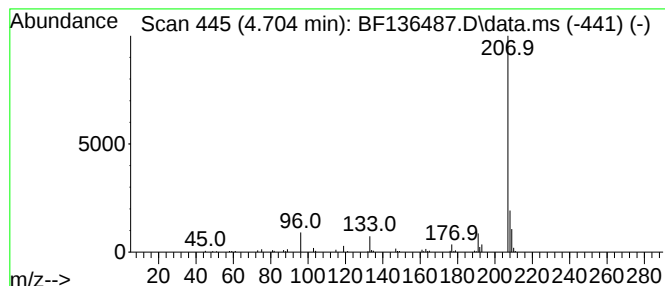
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Cyclotrisiloxane, hexamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.704	2.13 ng	82988	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	90
2			Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	45
3			4-tert-Octylphenol, TMS derivative	278	C17H30OSi	078721-87-6	39
4			1H-Indole, 5-methyl-2-phenyl-	207	C15H13N	013228-36-9	38
5			2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	38



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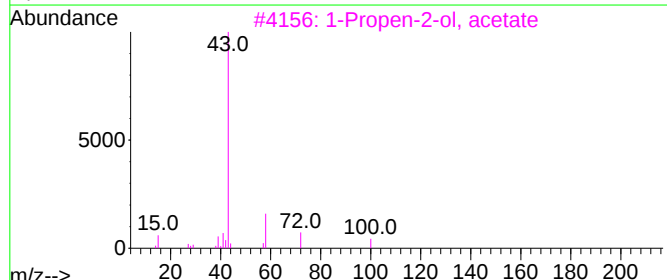
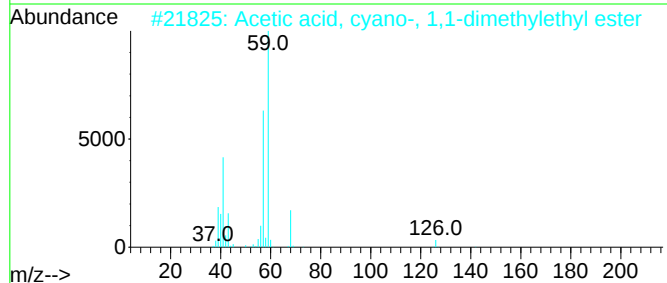
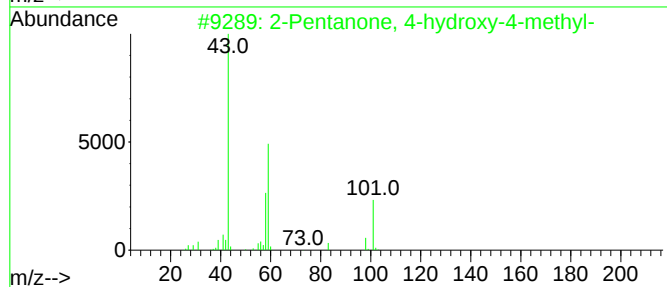
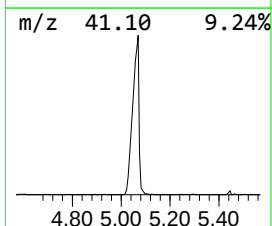
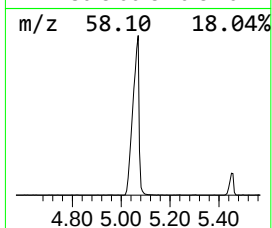
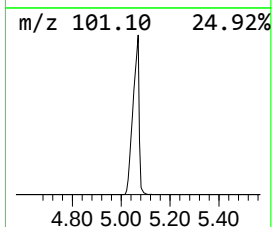
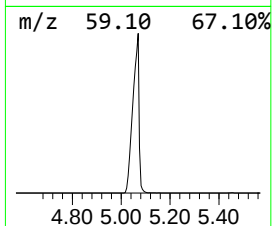
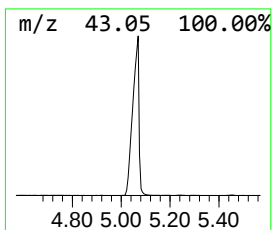
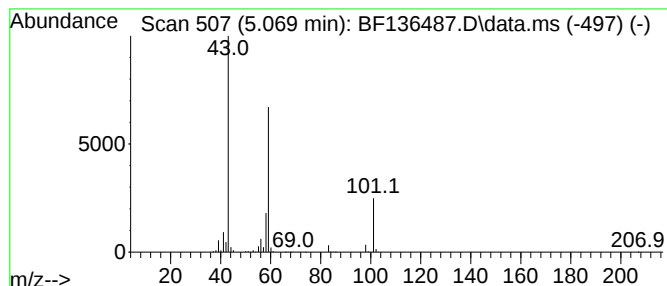
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.069	96.56 ng	3757060	1,4-Dichlorobenzene-d4			6.793
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
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	Butane, 1-ethoxy-	102	C6H14O		000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9



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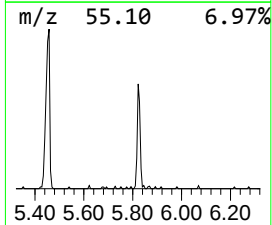
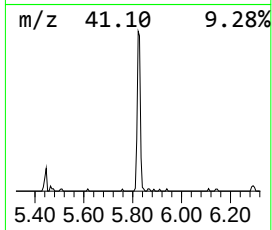
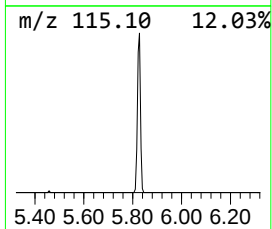
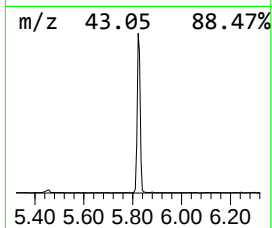
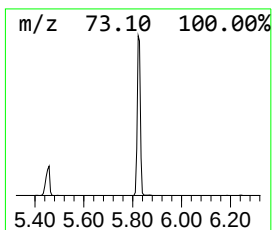
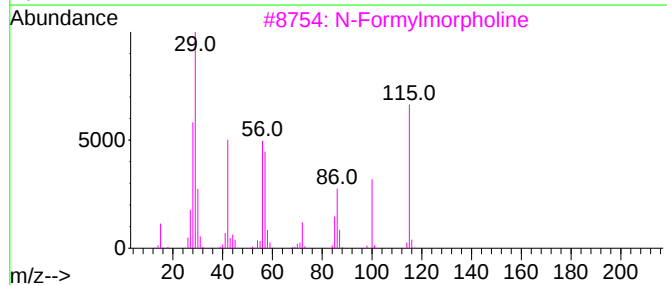
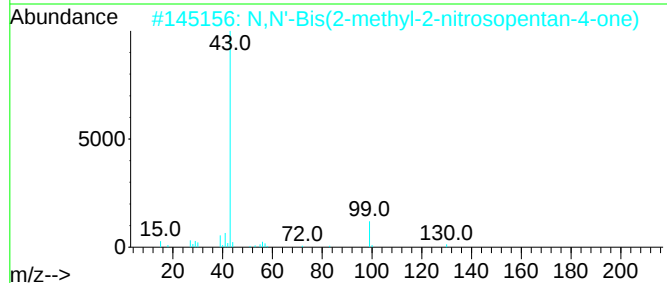
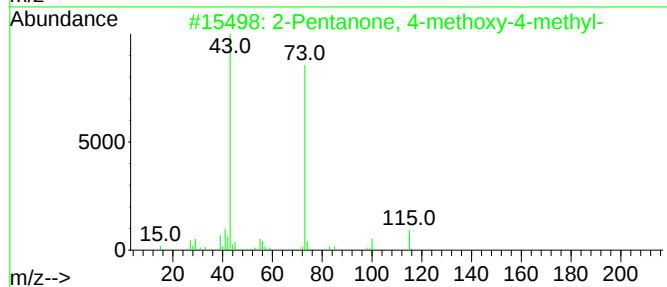
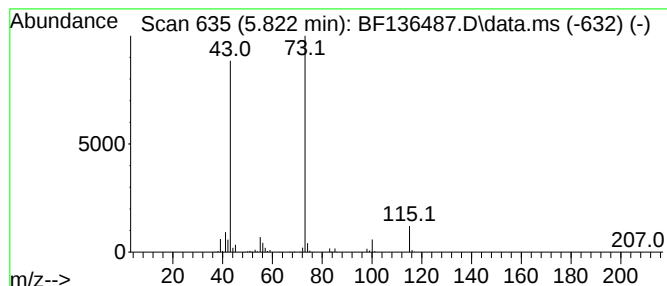
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.822	8.41 ng	327358	1,4-Dichlorobenzene-d4	6.793	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
3	N-Formylmorpholine	115	C5H9NO2	004394-85-8	9
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9



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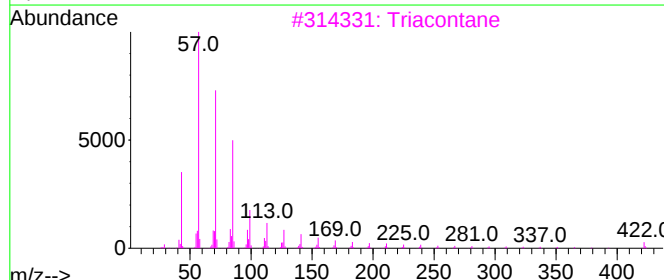
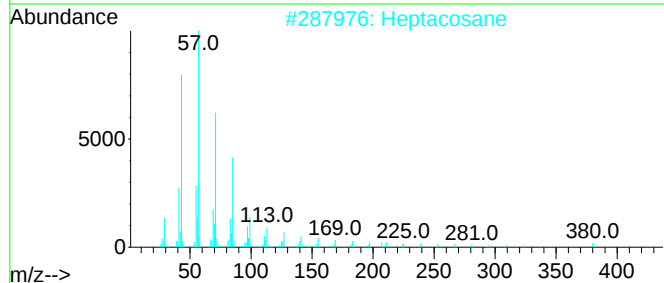
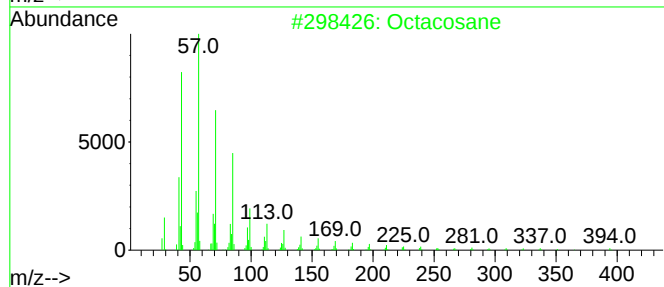
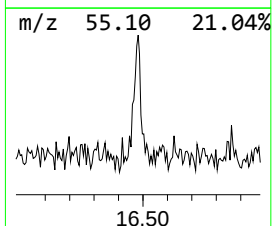
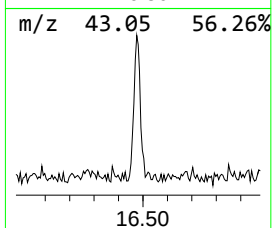
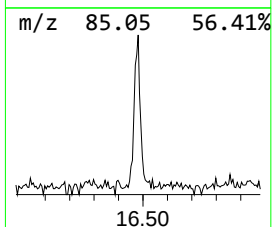
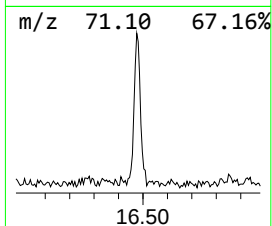
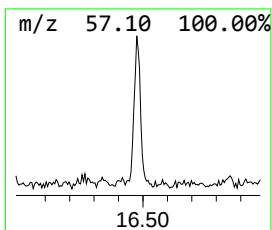
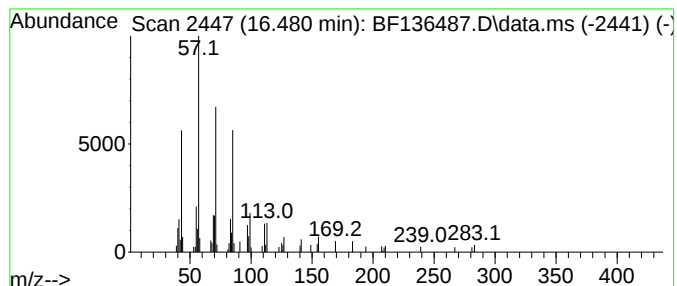
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	2.14 ng	79322	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Triacontane	422	C30H62	000638-68-6	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Heneicosane	296	C21H44	000629-94-7	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.463	149.7	ng	5823590	1	6.793	778209	20.0
Cyclotrisiloxan...	4.704	2.1	ng	82988	1	6.793	778209	20.0
2-Pentanone, 4-...	5.069	96.6	ng	3757060	1	6.793	778209	20.0
2-Pentanone, 4-...	5.822	8.4	ng	327358	1	6.793	778209	20.0
Octacosane	16.480	2.1	ng	79322	6	15.451	740213	20.0