

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
 Data File : BF133984.D
 Acq On : 27 Jun 2023 11:03
 Operator : CG\JU
 Sample : PB153762BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB153762BL

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: BF133984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.493	405	409	421	rBV	214869	246816	5.82%	0.966%
2	5.104	507	513	525	rBV	1003899	1386161	32.71%	5.426%
3	5.498	574	580	583	rBV	3038214	3036357	71.64%	11.885%
4	6.493	743	749	751	rBV	2567371	3089745	72.90%	12.094%
5	6.851	806	810	813	rBV	738798	632706	14.93%	2.476%
6	7.416	900	906	909	rBV	2156940	2024719	47.77%	7.925%
7	8.128	1023	1027	1040	rBV	1051418	856136	20.20%	3.351%
8	9.210	1205	1211	1214	rBV	4362263	3729129	87.99%	14.596%
9	9.886	1322	1326	1330	rBV	1212299	971814	22.93%	3.804%
10	10.681	1457	1461	1465	rBV	2577032	2651455	62.56%	10.378%
11	11.380	1576	1580	1588	rBV	1274507	1099413	25.94%	4.303%
12	12.986	1847	1853	1856	rBV	4067299	4238263	100.00%	16.589%
13	14.039	2028	2032	2040	rVB	863546	798273	18.83%	3.125%
14	15.545	2283	2288	2293	rBV2	467964	611907	14.44%	2.395%
15	16.045	2369	2373	2381	rVB2	27794	43948	1.04%	0.172%
16	16.586	2460	2465	2472	rBV3	33585	65336	1.54%	0.256%
17	17.227	2569	2574	2585	rVB6	24983	66227	1.56%	0.259%

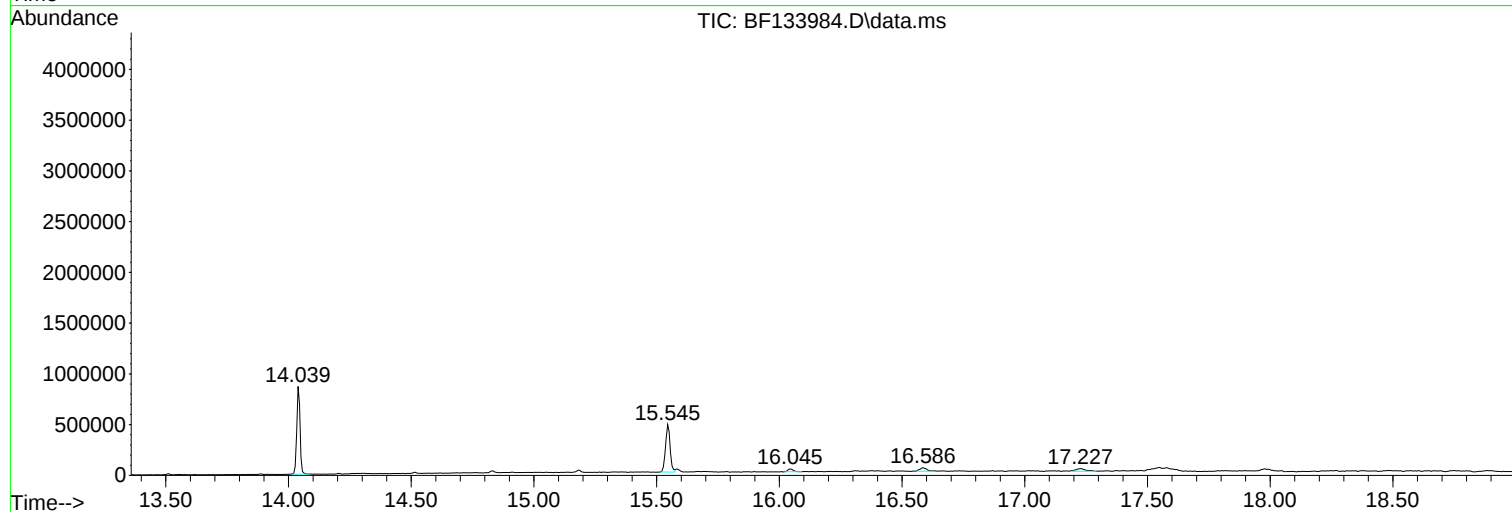
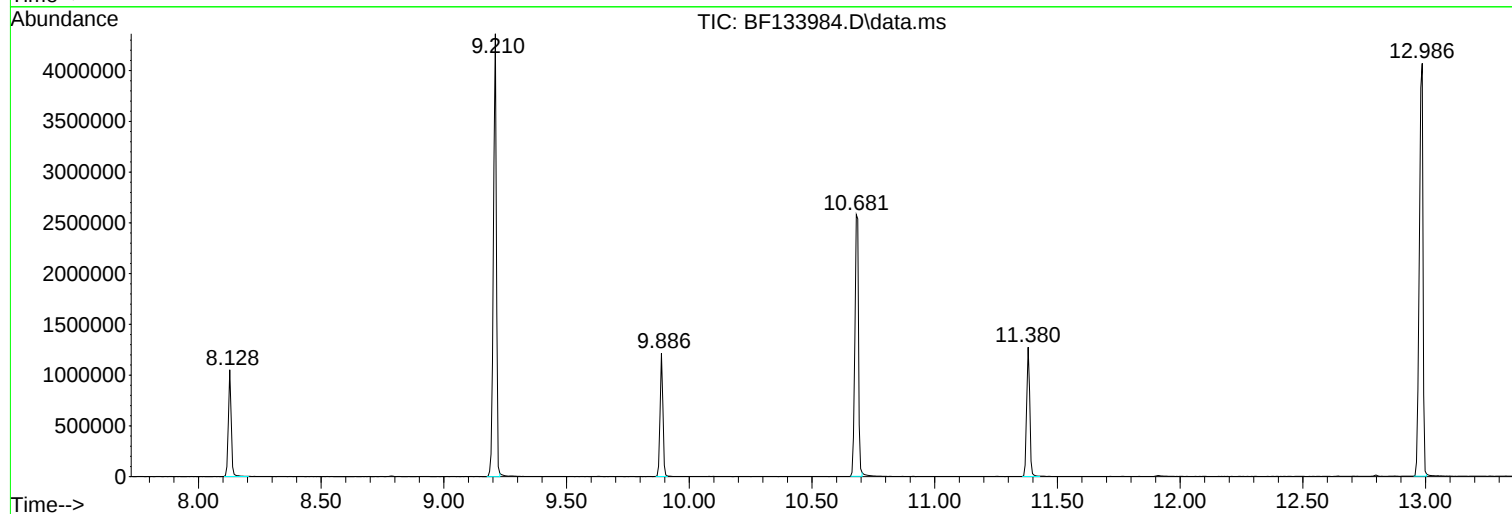
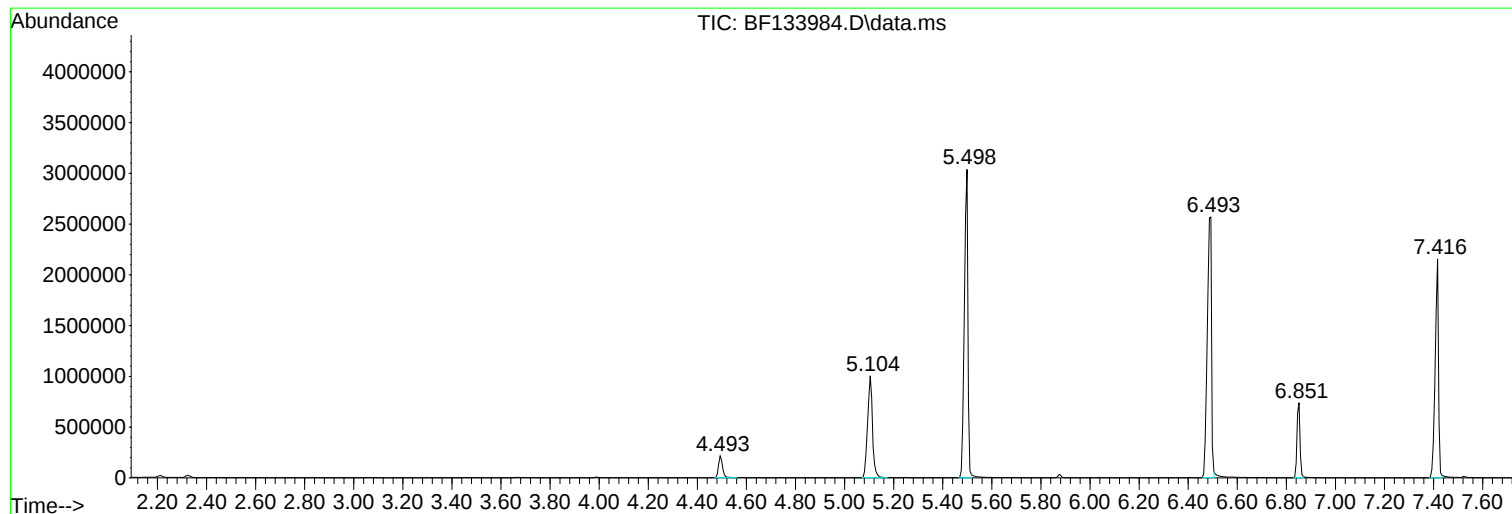
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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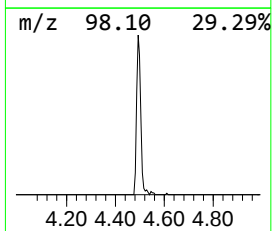
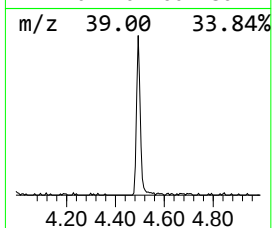
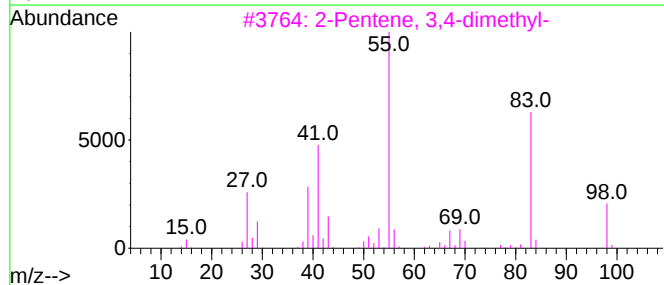
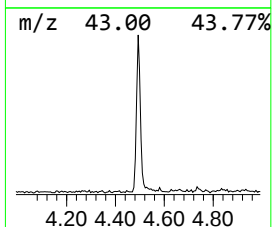
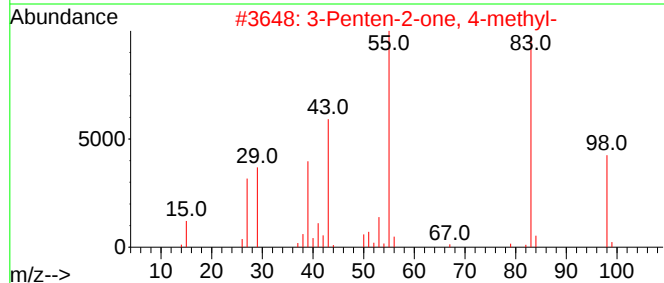
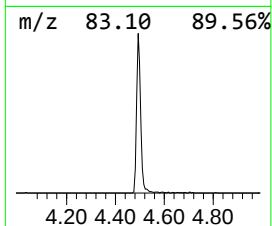
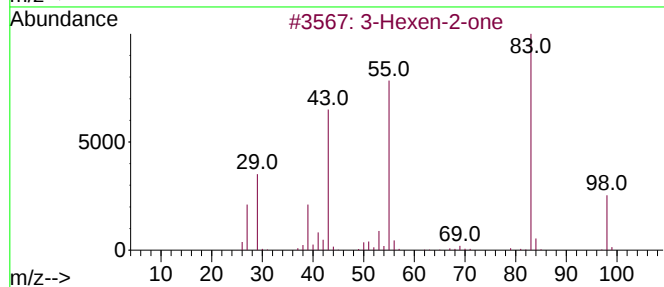
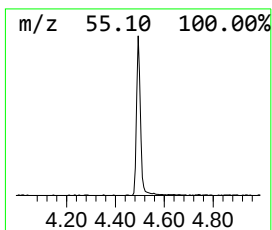
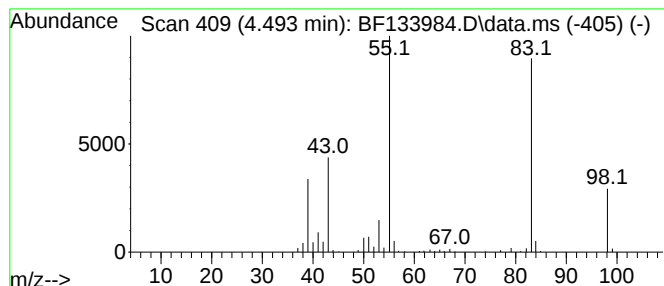
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.493	7.80 ng	246816	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one			98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-			98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-			98	C7H14	024910-63-2	86
4	2-Pentene, 4,4-dimethyl-, (E)-			98	C7H14	000690-08-4	78
5	2-Pentene, 2,4-dimethyl-			98	C7H14	000625-65-0	78



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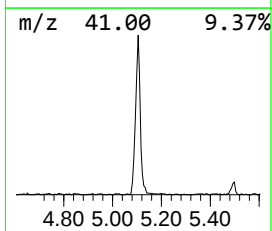
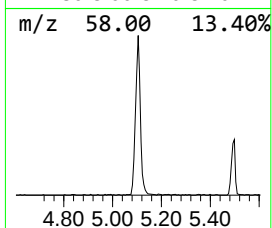
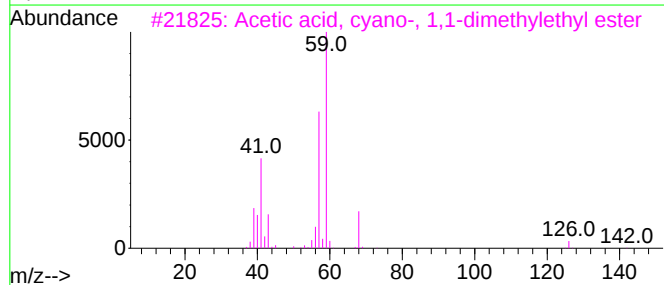
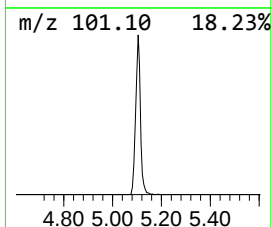
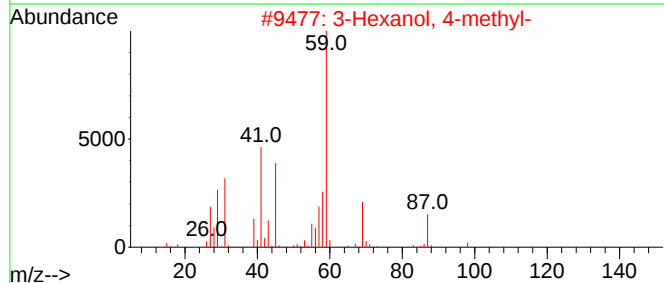
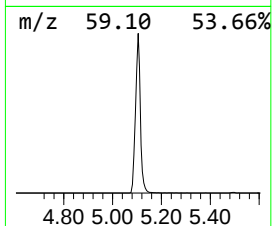
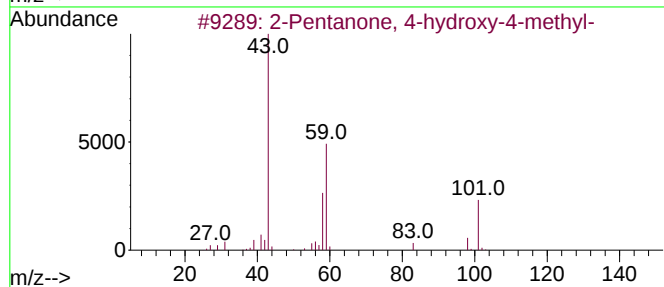
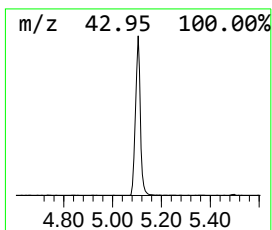
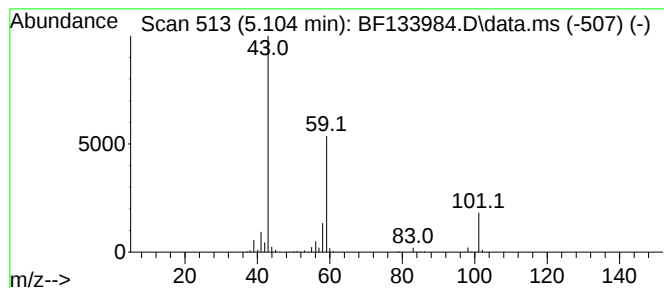
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.104	43.82 ng	1386160	1,4-Dichlorobenzene-d4			6.851

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	12



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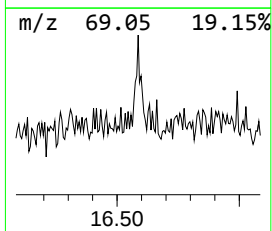
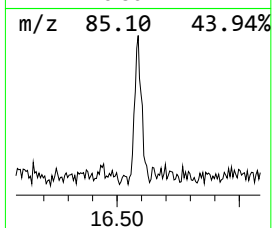
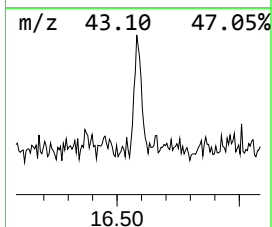
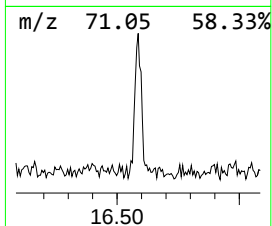
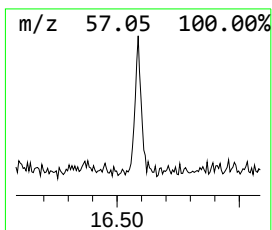
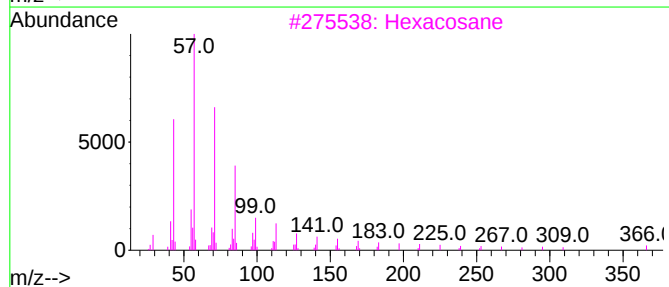
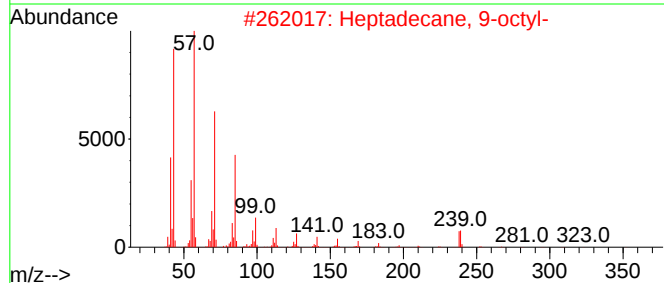
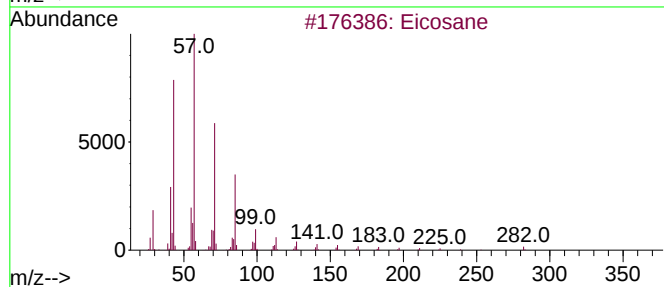
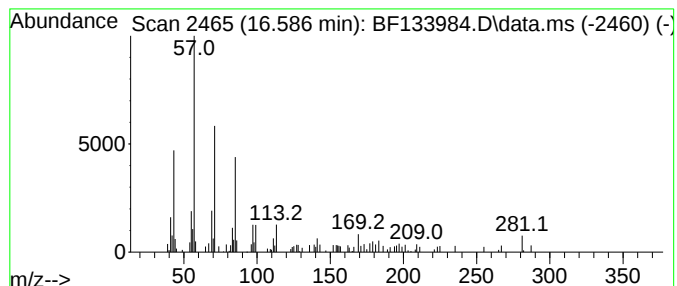
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Peak Number 3 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	2.14 ng	65336	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	87
2	Heptadecane, 9-octyl-			352	C25H52	007225-64-1	86
3	Hexacosane			366	C26H54	000630-01-3	86
4	Eicosane, 7-hexyl-			366	C26H54	055333-99-8	86
5	Dotriacontane, 1-iodo-			576	C32H65I	1000406-32-4	80



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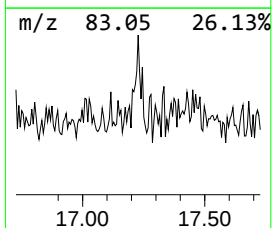
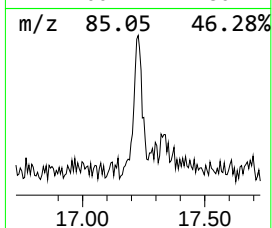
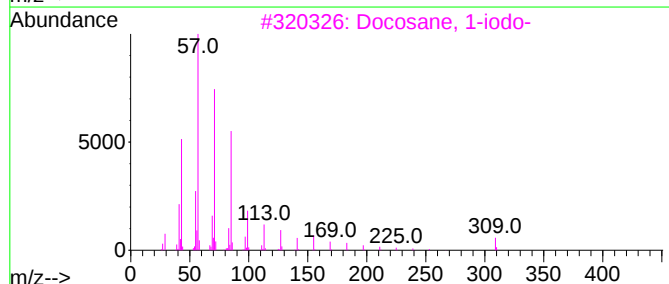
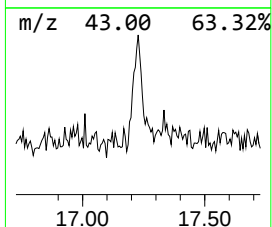
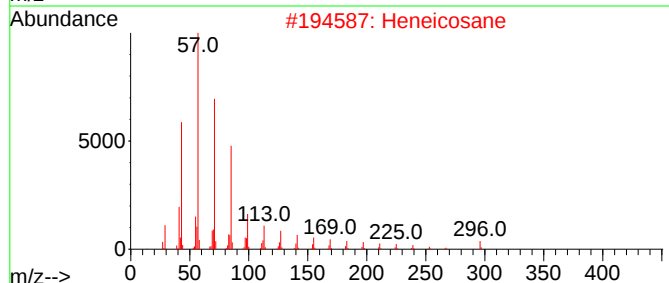
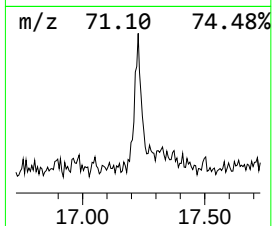
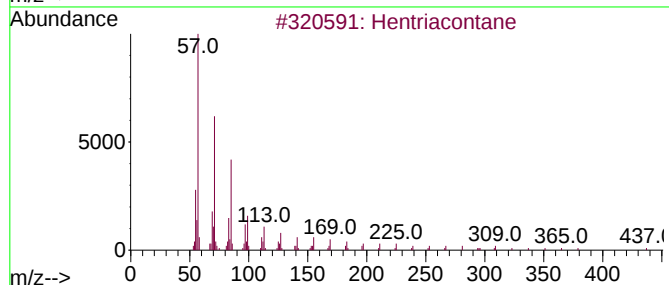
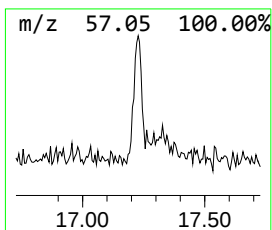
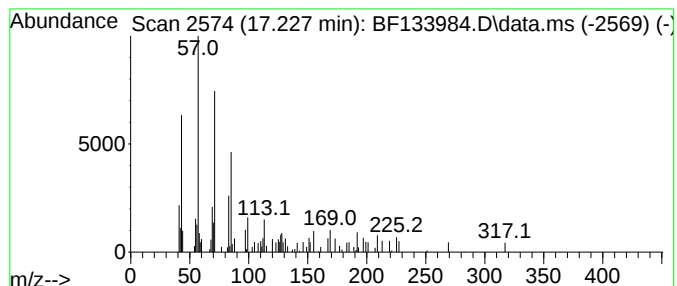
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Peak Number 4 Hentriacontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.227	2.16 ng	66227	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	80
2			Heneicosane	296	C21H44	000629-94-7	72
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	72
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
5			11-Methylpentacosane	366	C26H54	015689-71-1	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.493	7.8	ng	246816	1	6.851	632706	20.0
2-Pentanone, 4-...	5.104	43.8	ng	1386160	1	6.851	632706	20.0
Eicosane	16.586	2.1	ng	65336	6	15.545	611907	20.0
Hentriacontane	17.227	2.2	ng	66227	6	15.545	611907	20.0