

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122821\
 Data File : BF126382.D
 Acq On : 28 Dec 2021 15:33
 Operator : JU/CG
 Sample : M5187-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2-119-1-5-10

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.857	296	301	308	rVB	16219	24011	1.07%	0.147%
2	5.016	491	498	504	rBV	215813	269597	12.04%	1.653%
3	5.422	562	567	570	rBV	2213048	2124468	94.84%	13.024%
4	6.440	734	740	743	rBV	2154456	2239943	100.00%	13.732%
5	6.810	799	803	806	rBV	836120	668364	29.84%	4.097%
6	7.369	893	898	901	rBV	1578906	1480811	66.11%	9.078%
7	8.092	1016	1021	1027	rBV	1018403	886389	39.57%	5.434%
8	8.692	1119	1123	1125	rBV	32179	28721	1.28%	0.176%
9	9.169	1200	1204	1207	rBV	2476496	2151621	96.06%	13.190%
10	9.257	1215	1219	1224	rVB2	59266	58197	2.60%	0.357%
11	9.786	1304	1309	1313	rVB	26786	24418	1.09%	0.150%
12	9.845	1315	1319	1329	rVB	990051	879284	39.25%	5.390%
13	10.257	1386	1389	1392	rBV2	21285	23675	1.06%	0.145%
14	10.633	1449	1453	1463	rBV	1196951	1066816	47.63%	6.540%
15	11.204	1542	1550	1553	rBV5	24844	46049	2.06%	0.282%
16	11.298	1562	1566	1568	rBV	28381	25092	1.12%	0.154%
17	11.333	1568	1572	1575	rBV	837596	748298	33.41%	4.587%
18	11.498	1597	1600	1607	rVB	26286	31257	1.40%	0.192%
19	11.898	1665	1668	1670	rVB	52980	40299	1.80%	0.247%
20	12.316	1734	1739	1742	rBV	32130	31312	1.40%	0.192%
21	12.369	1746	1748	1753	rVB	38883	38310	1.71%	0.235%
22	12.769	1811	1816	1819	rVB3	19838	29166	1.30%	0.179%
23	12.921	1837	1842	1845	rBV	1671747	1571094	70.14%	9.631%
24	13.539	1942	1947	1950	rVB	29176	24515	1.09%	0.150%
25	13.574	1950	1953	1957	rVB	30018	28296	1.26%	0.173%
26	13.874	1998	2004	2005	rBV4	33759	63714	2.84%	0.391%
27	13.968	2015	2020	2024	rBV	646119	622440	27.79%	3.816%
28	14.451	2099	2102	2106	rBV2	28595	30282	1.35%	0.186%
29	14.757	2151	2154	2157	rVB	38603	35134	1.57%	0.215%
30	14.827	2163	2166	2172	rBV	55969	61090	2.73%	0.375%
31	15.086	2206	2210	2215	rBV	57431	80100	3.58%	0.491%
32	15.421	2262	2267	2271	rBV	540597	724350	32.34%	4.441%
33	15.457	2271	2273	2279	rVB	50073	70727	3.16%	0.434%
34	15.886	2343	2346	2351	rVB2	35504	49425	2.21%	0.303%
35	16.386	2424	2431	2437	rBV5	13738	34968	1.56%	0.214%

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ClientSampleId :
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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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

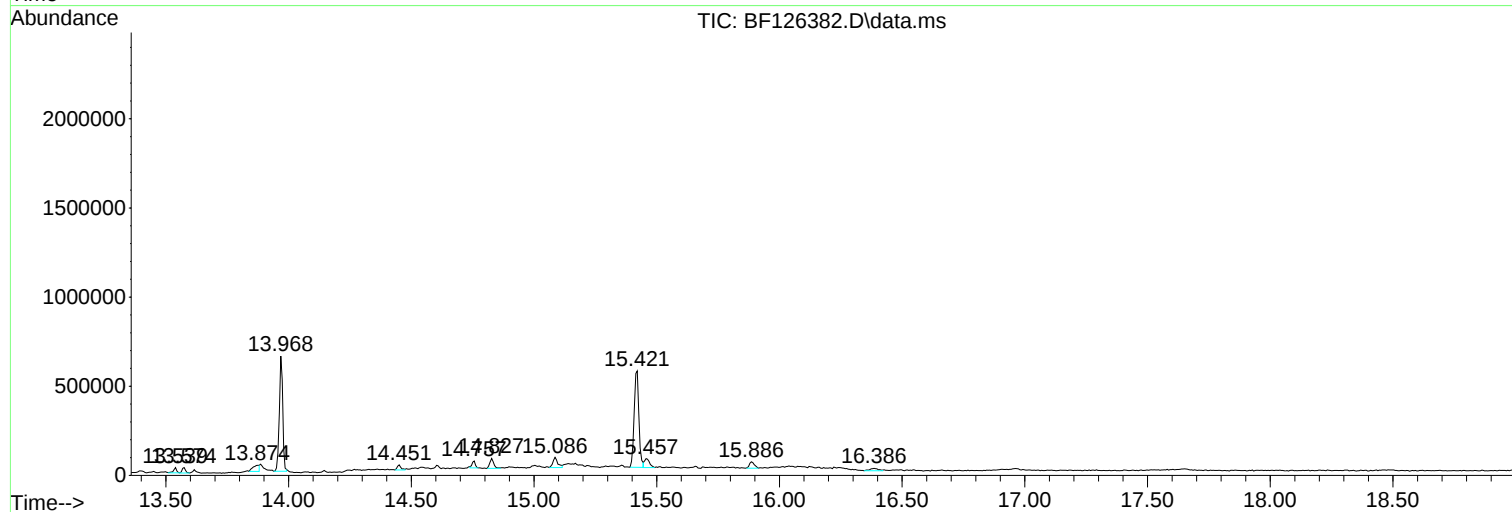
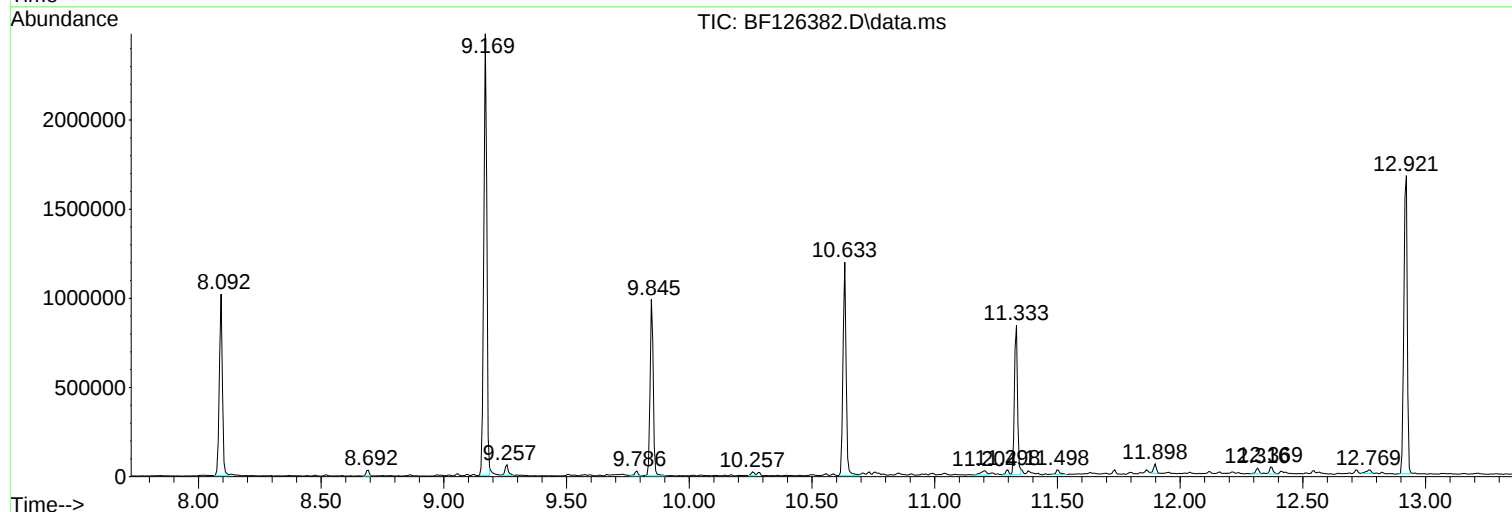
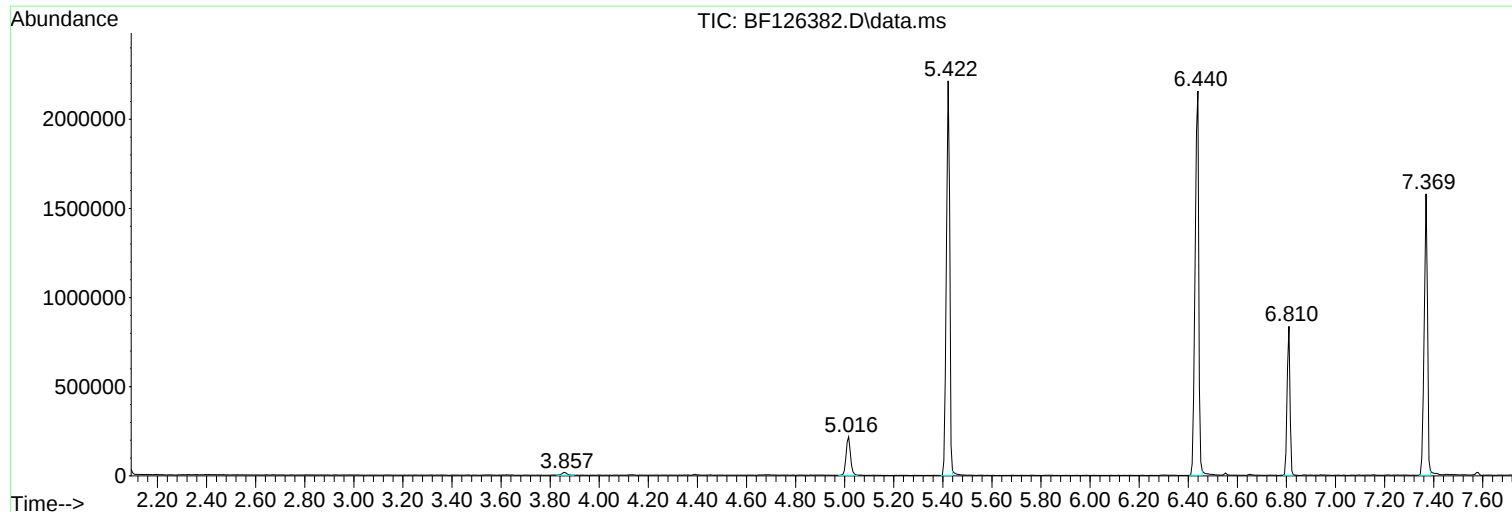
Sum of corrected areas: 16312233

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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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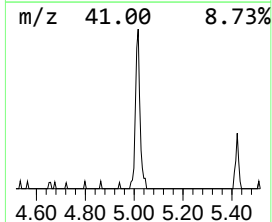
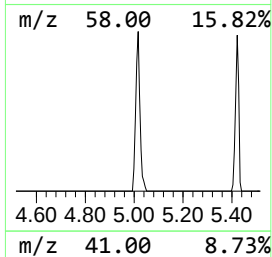
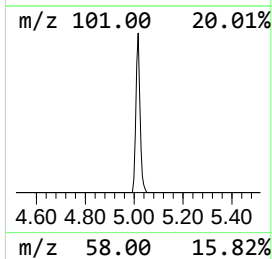
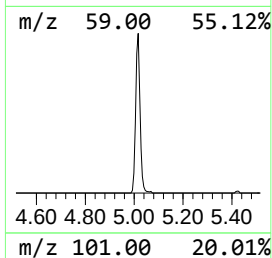
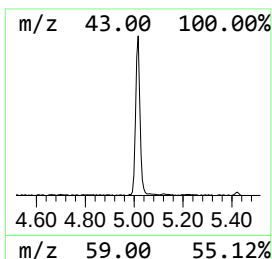
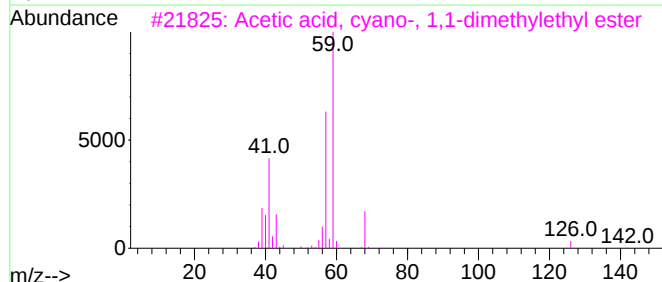
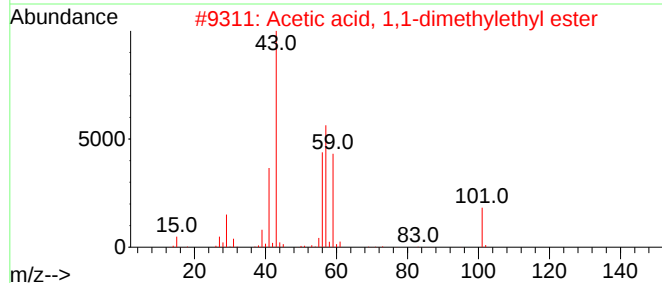
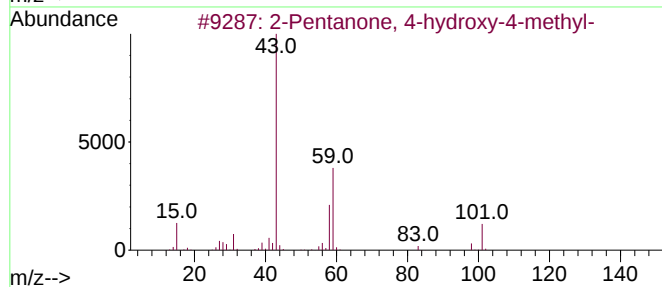
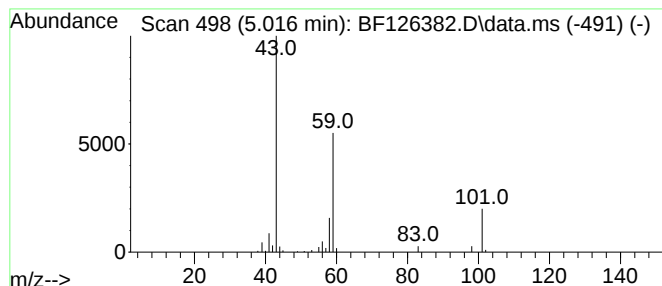
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.016	8.07 ng	269597	1,4-Dichlorobenzene-d4	6.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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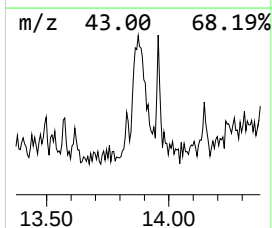
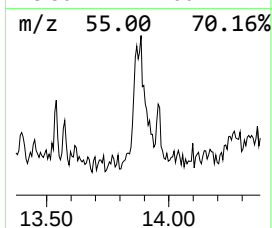
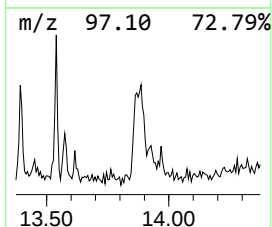
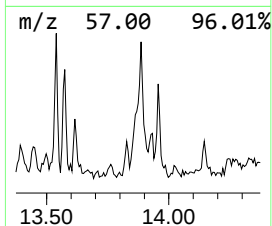
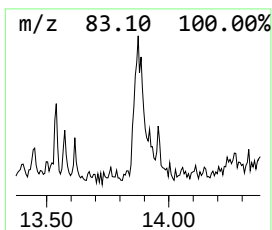
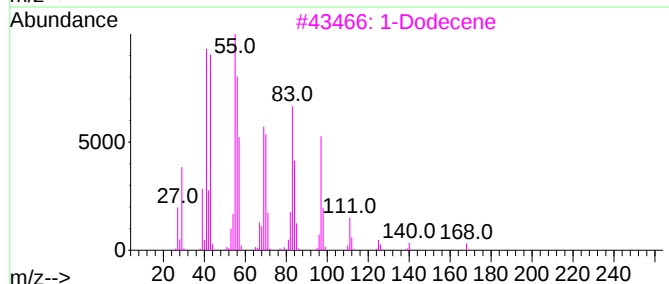
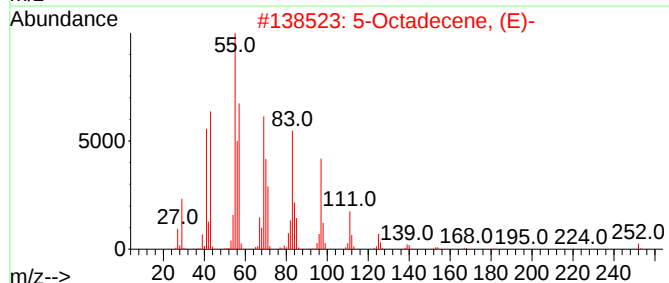
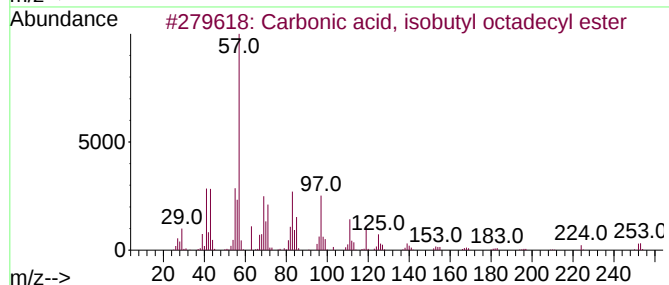
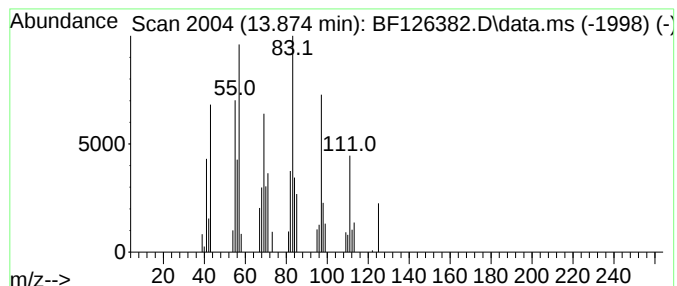
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Peak Number 2 Carbonic acid, isobutyl oct... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.05 ng	63714	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	53
2			5-Octadecene, (E)-	252	C18H36	007206-21-5	53
3			1-Dodecene	168	C12H24	000112-41-4	50
4			Butyl docosyl ether	382	C26H54O	1000406-40-8	47
5			Butyl tetracosyl ether	410	C28H58O	1000406-40-9	47



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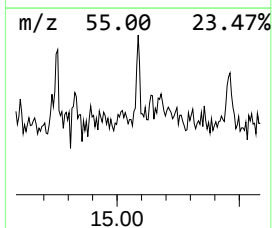
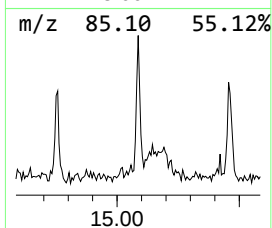
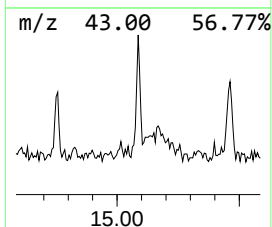
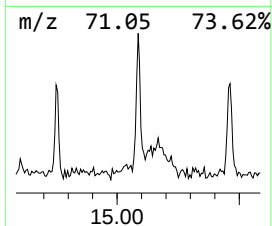
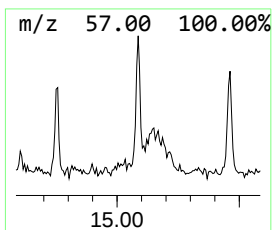
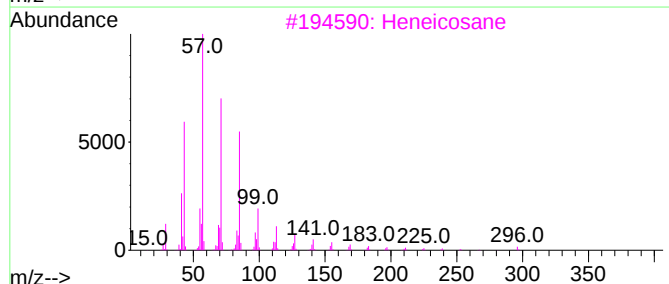
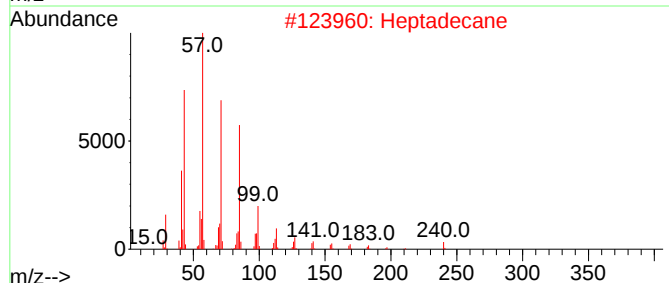
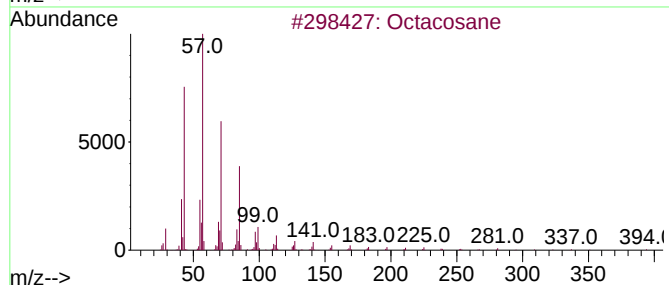
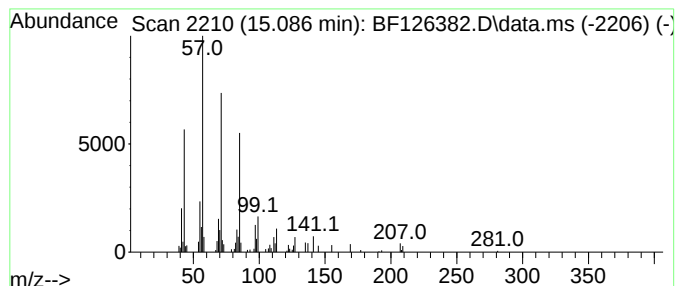
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.086	2.21 ng	80100	Perylene-d12	15.421	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Hexacosane	366	C26H54	000630-01-3	90



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	8.1	ng	269597	1	6.810	668364	20.0
Carbonic acid, ...	13.874	2.0	ng	63714	5	13.968	622440	20.0
Octacosane	15.086	2.2	ng	80100	6	15.421	724350	20.0