

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081123\
 Data File : BF134733.D
 Acq On : 11 Aug 2023 15:29
 Operator : CG\JU
 Sample : 03971-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-PP01A

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134733.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	13	16	21	rVB3	30810	38028	1.32%	0.163%
2	3.528	238	245	254	rVB	38257	66636	2.32%	0.285%
3	4.416	390	396	400	rBV	1928087	2206523	76.70%	9.438%
4	5.028	495	500	513	rVB	784229	831690	28.91%	3.558%
5	5.428	564	568	572	rBV	2110096	1975672	68.68%	8.451%
6	6.292	712	715	719	rBV	39543	31488	1.09%	0.135%
7	6.434	734	739	742	rBV	2806239	2501581	86.96%	10.700%
8	6.628	769	772	781	rBV	71553	81429	2.83%	0.348%
9	6.798	797	801	808	rVB	1328536	1041668	36.21%	4.456%
10	6.863	808	812	819	rVV	33987	46252	1.61%	0.198%
11	6.922	819	822	829	rVB	26496	30895	1.07%	0.132%
12	7.357	890	896	899	rBV	1988343	1779259	61.85%	7.611%
13	8.075	1014	1018	1025	rBV	1530545	1289336	44.82%	5.515%
14	9.098	1190	1192	1195	rVB	44679	38256	1.33%	0.164%
15	9.151	1197	1201	1210	rBV	3156710	2876711	100.00%	12.305%
16	9.233	1212	1215	1219	rVV	105871	103259	3.59%	0.442%
17	9.275	1219	1222	1225	rVB2	46178	45569	1.58%	0.195%
18	9.557	1265	1270	1272	rBV3	80441	89236	3.10%	0.382%
19	9.769	1303	1306	1309	rBV	133581	94847	3.30%	0.406%
20	9.833	1313	1317	1322	rVB	1299382	1127067	39.18%	4.821%
21	10.269	1388	1391	1394	rVB	75562	55613	1.93%	0.238%
22	10.492	1424	1429	1434	rBV	38274	42486	1.48%	0.182%
23	10.616	1447	1450	1464	rVB	845949	792390	27.54%	3.389%
24	10.757	1469	1474	1481	rVB	65858	94003	3.27%	0.402%
25	11.321	1566	1570	1573	rBV	1203171	1027970	35.73%	4.397%
26	11.851	1656	1660	1665	rBV	118586	137436	4.78%	0.588%
27	12.645	1791	1795	1804	rBV7	24501	40695	1.41%	0.174%
28	12.915	1837	1841	1844	rBV	2969603	2643494	91.89%	11.307%
29	13.498	1934	1940	1942	rBV2	30803	35528	1.24%	0.152%
30	13.827	1992	1996	2003	rBV	182542	217662	7.57%	0.931%
31	13.968	2015	2020	2030	rBV	1096625	1103231	38.35%	4.719%
32	14.145	2047	2050	2054	rBV	36882	37806	1.31%	0.162%
33	14.451	2100	2102	2110	rBV4	34098	57555	2.00%	0.246%
34	14.762	2152	2155	2161	rBV	29322	37095	1.29%	0.159%
35	14.839	2164	2168	2172	rVB	44717	48930	1.70%	0.209%
36	15.439	2265	2270	2277	rBV	565316	711097	24.72%	3.042%

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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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

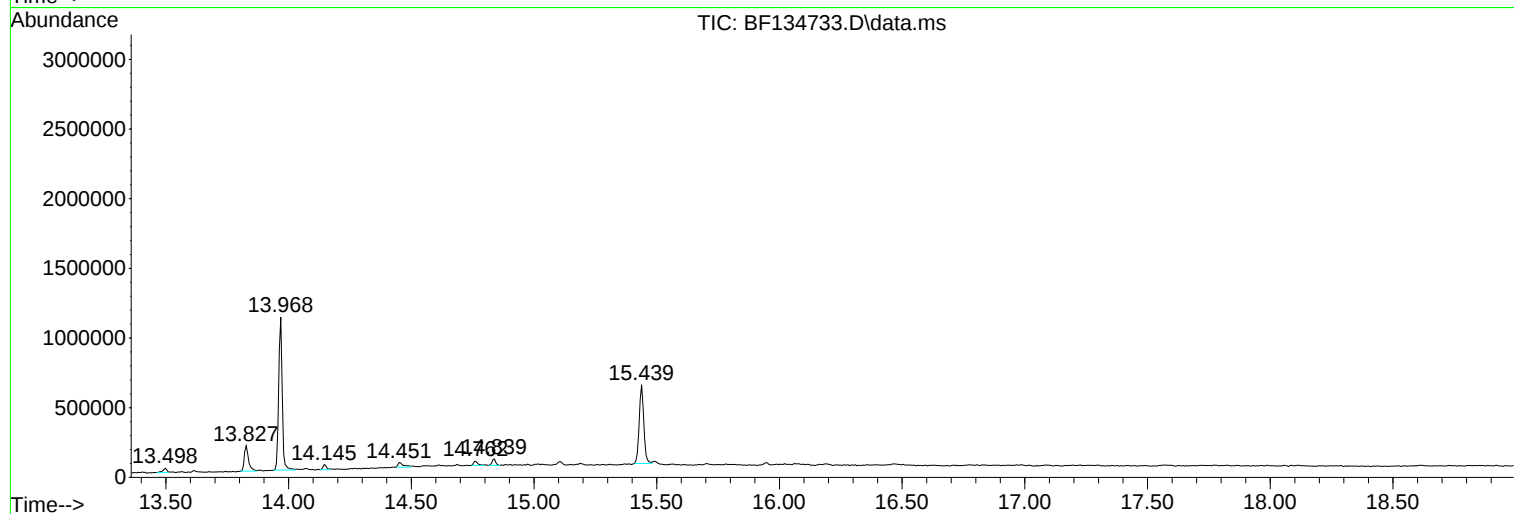
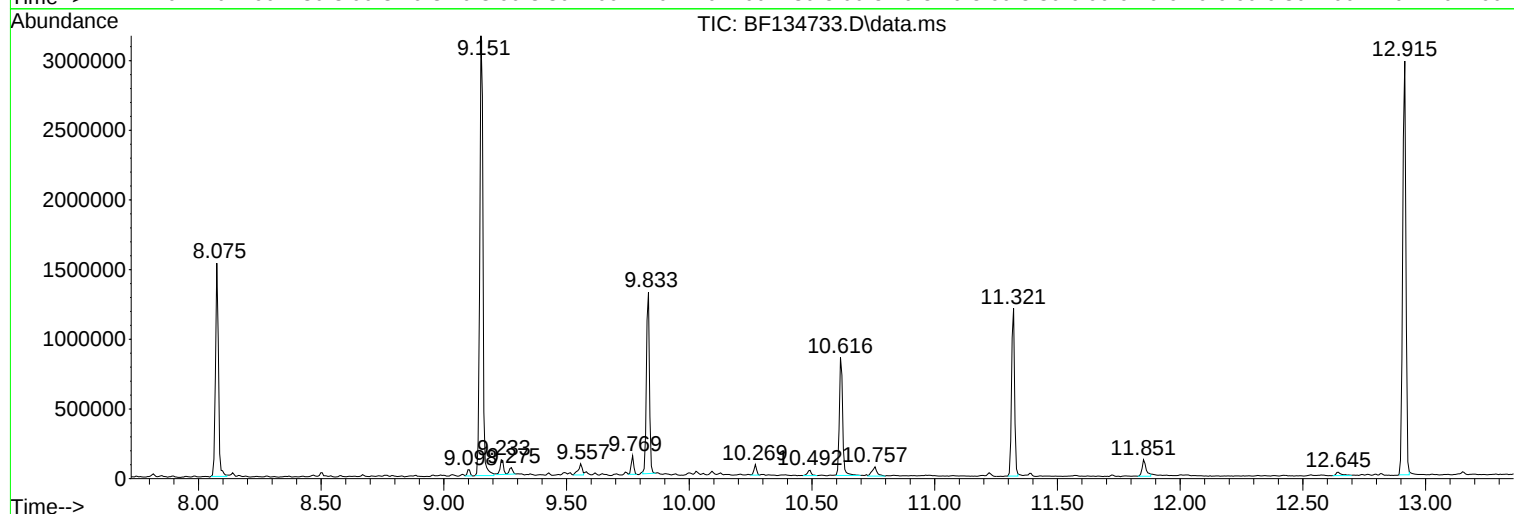
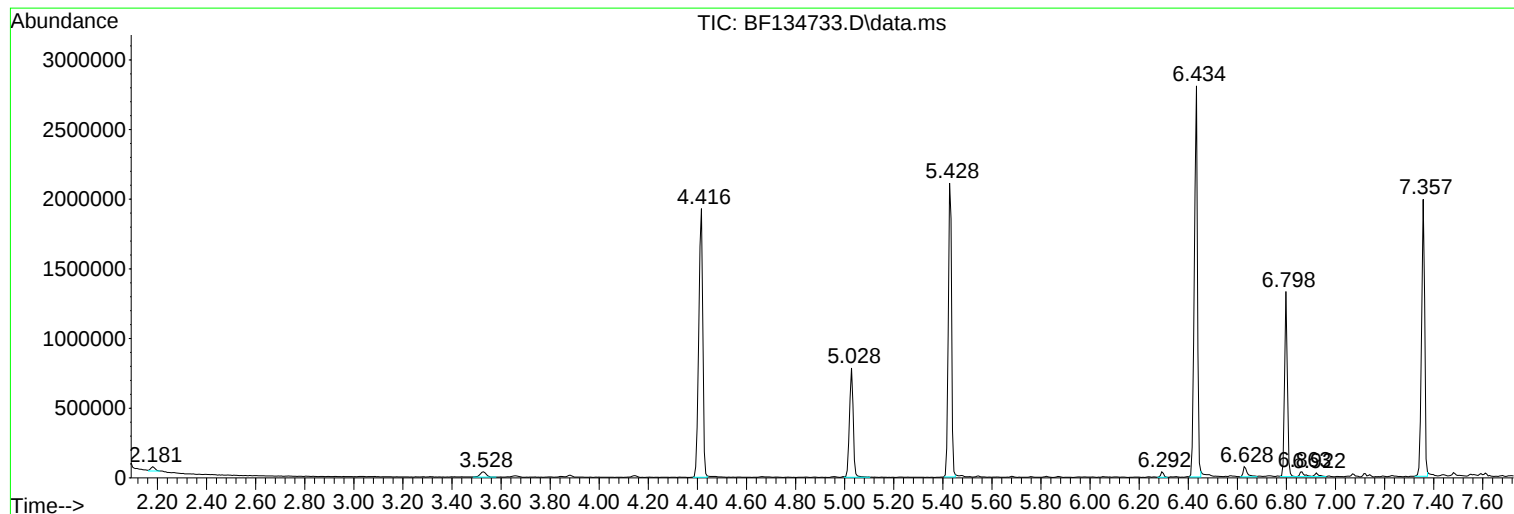
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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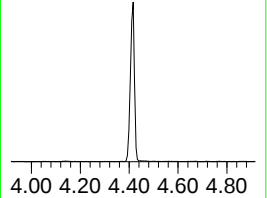
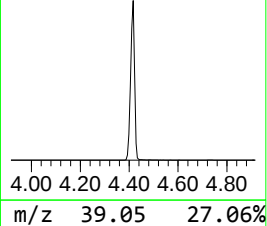
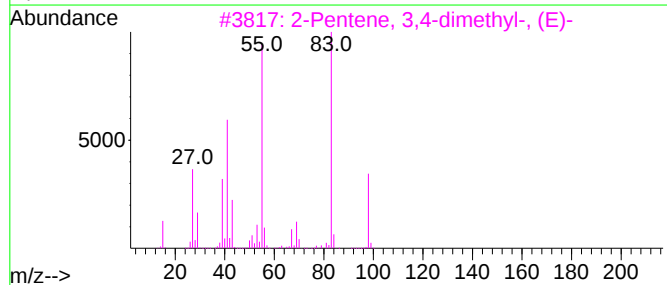
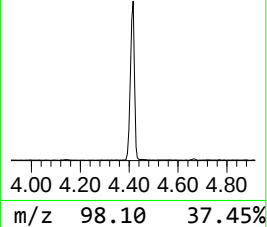
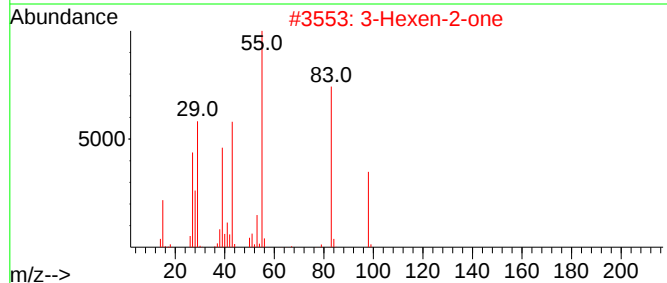
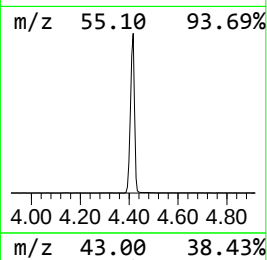
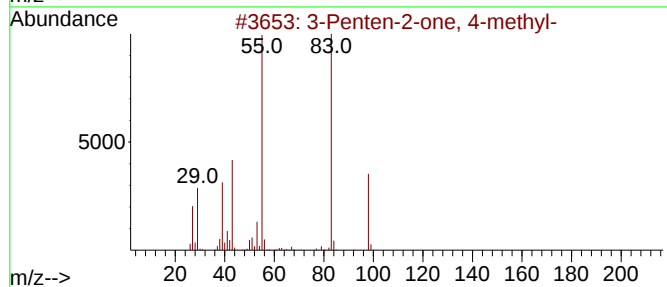
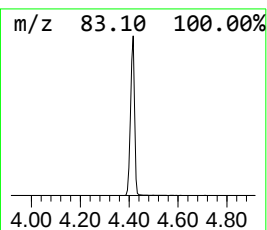
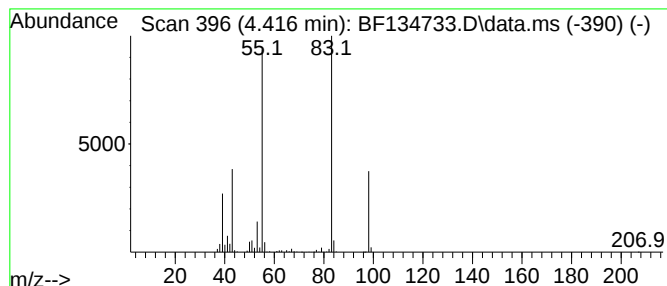
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.416	42.37 ng	2206520	1,4-Dichlorobenzene-d4	6.798

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, 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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Instrument :
BNA_F
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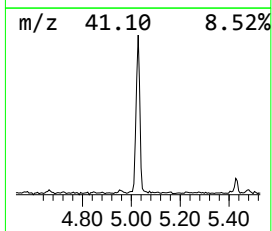
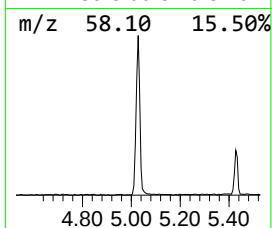
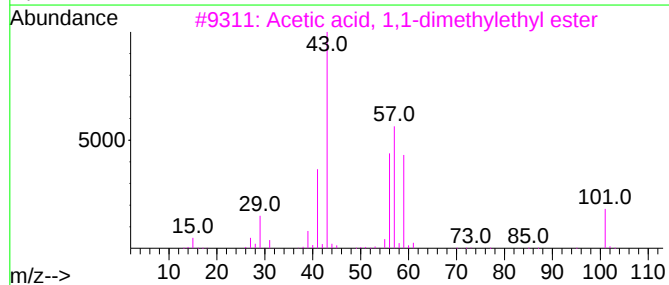
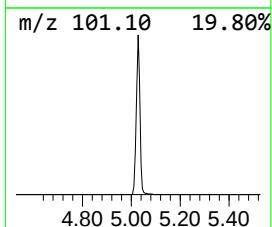
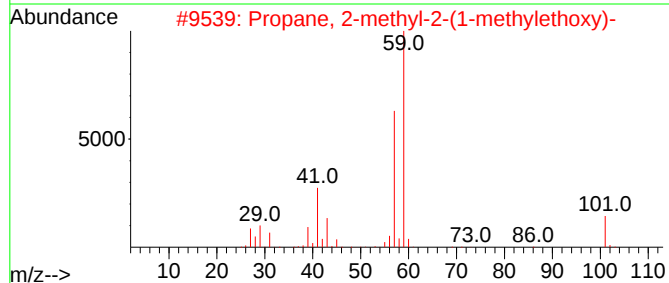
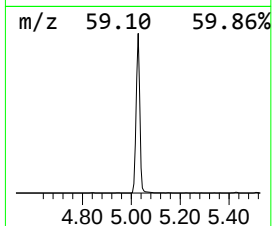
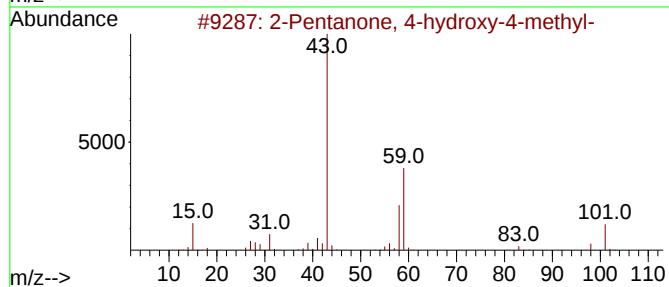
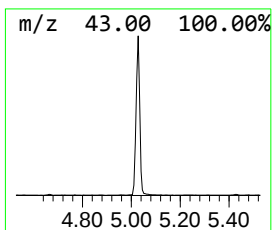
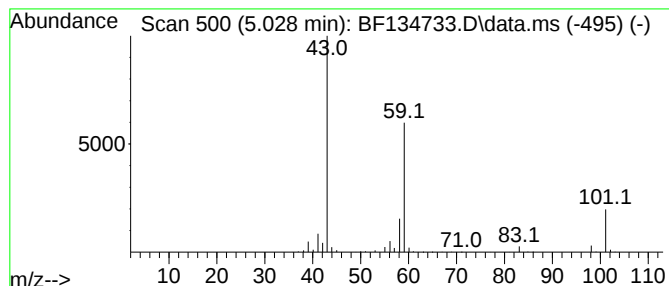
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	15.97 ng	831690	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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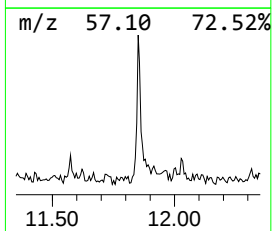
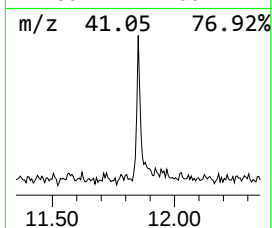
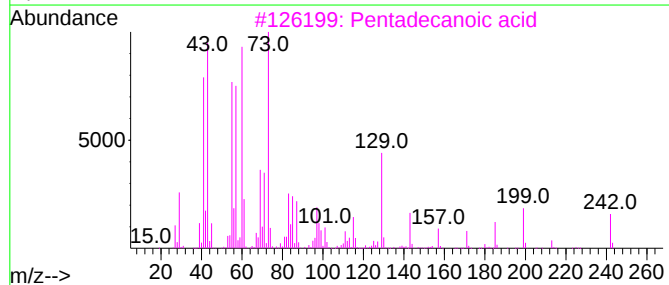
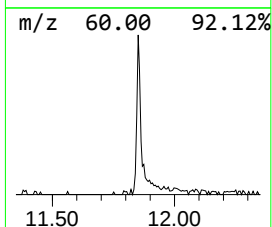
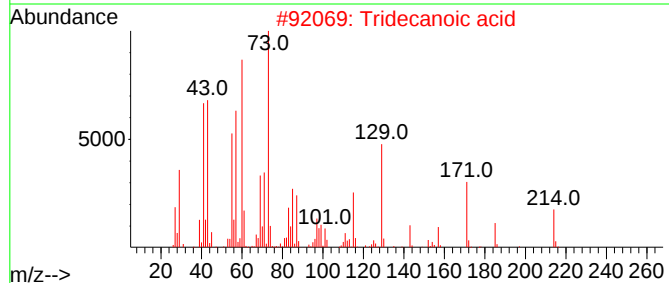
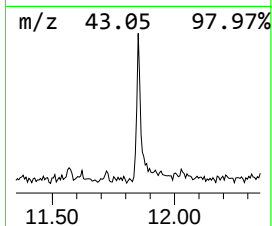
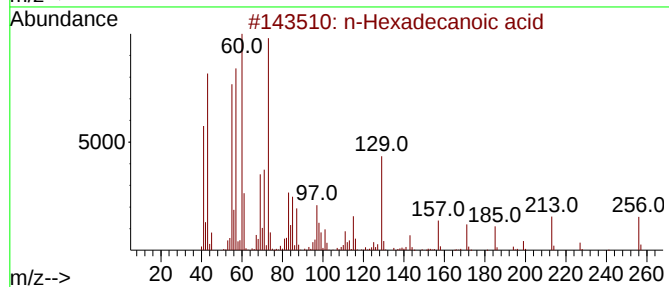
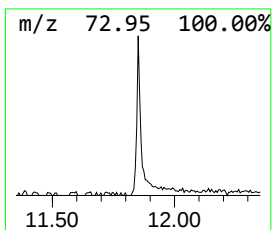
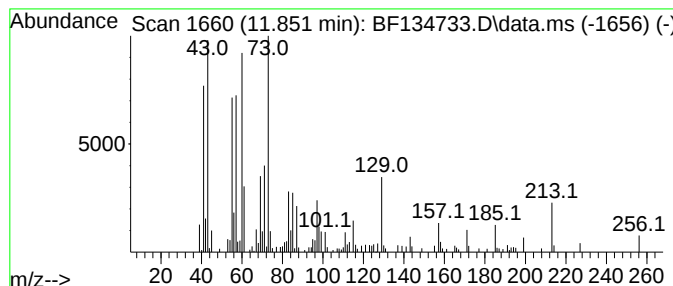
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	2.67 ng	137436	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	46



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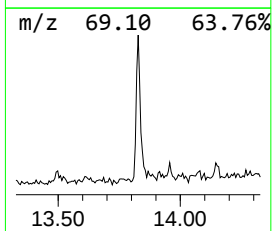
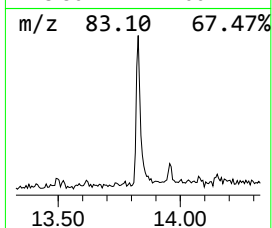
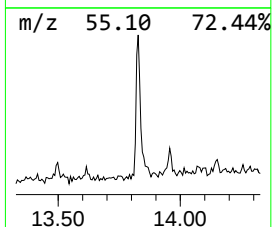
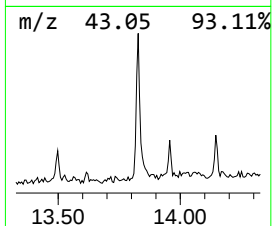
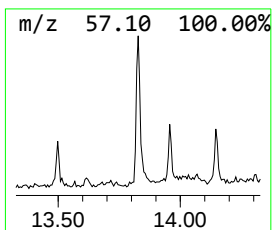
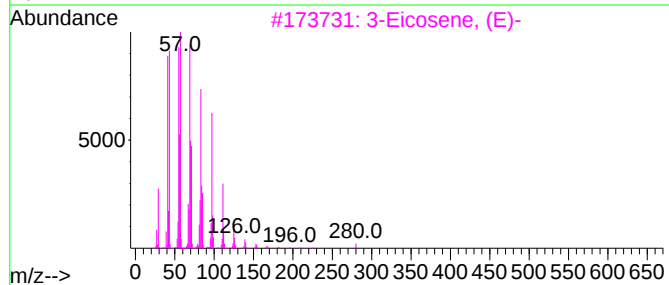
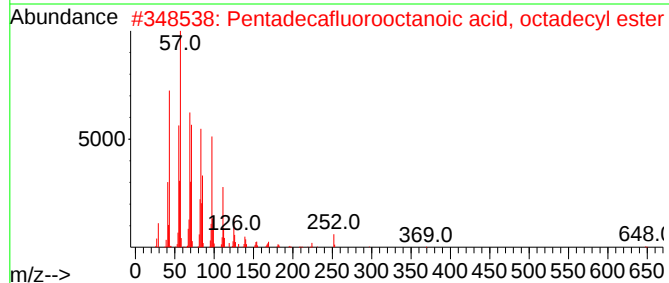
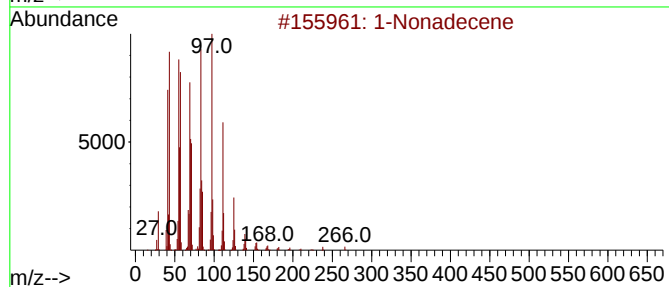
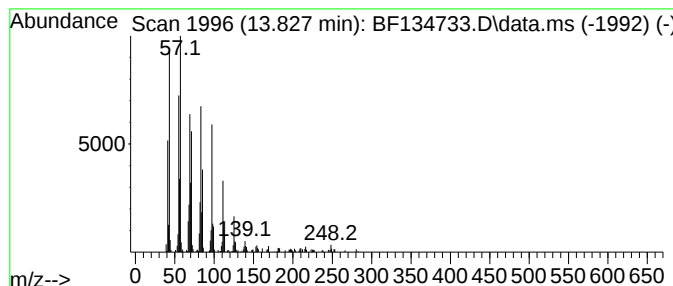
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	3.95 ng	217662	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	98
2	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	94
3	3-Eicosene, (E)-			280	C20H40	074685-33-9	93
4	1-Hexadecanesulfonyl chloride			324	C16H33ClO2S	038775-38-1	91
5	1-Hexacosene			364	C26H52	018835-33-1	91



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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
3-Penten-2-one,...	4.416	42.4	ng	2206520	1	6.798	1041670	20.0
2-Pentanone, 4-...	5.028	16.0	ng	831690	1	6.798	1041670	20.0
n-Hexadecanoic ...	11.851	2.7	ng	137436	4	11.322	1027970	20.0
1-Nonadecene	13.827	4.0	ng	217662	5	13.968	1103230	20.0