

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030724\
 Data File : BF137527.D
 Acq On : 07 Mar 2024 13:41
 Operator : CG\JU
 Sample : PB159470BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159470BL

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137527.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	23	29	35	rVB	83009	119398	1.30%	0.215%
2	2.375	45	49	55	rBV	69143	99203	1.08%	0.179%
3	5.157	518	522	531	rBV	214603	335637	3.65%	0.606%
4	5.534	581	586	589	rBV	6173560	6690363	72.81%	12.073%
5	6.510	747	752	755	rBV	5780759	7040762	76.63%	12.706%
6	6.863	809	812	824	rBV	1721817	1547794	16.85%	2.793%
7	7.428	903	908	911	rBV	4375628	4486978	48.83%	8.097%
8	8.139	1024	1029	1051	rBV	2187772	2162945	23.54%	3.903%
9	9.222	1207	1213	1216	rBV	7807794	7788653	84.77%	14.055%
10	9.898	1323	1328	1343	rBV	2833762	2583554	28.12%	4.662%
11	10.698	1459	1464	1489	rBV	4600152	5134612	55.88%	9.266%
12	11.392	1578	1582	1591	rBV	2947438	2687272	29.25%	4.849%
13	12.668	1795	1799	1802	rBV	119285	97594	1.06%	0.176%
14	12.821	1822	1825	1829	rBV	346293	276698	3.01%	0.499%
15	13.004	1850	1856	1859	rBV	8715830	9188328	100.00%	16.581%
16	13.533	1943	1946	1951	rBV	218932	205749	2.24%	0.371%
17	14.057	2031	2035	2050	rBV	2124738	2130199	23.18%	3.844%
18	14.674	2132	2140	2149	rBV4	31422	103315	1.12%	0.186%
19	14.868	2170	2173	2180	rVB	107106	117332	1.28%	0.212%
20	15.239	2232	2236	2241	rVB	110087	136136	1.48%	0.246%
21	15.592	2290	2296	2304	rBV	1049778	1582943	17.23%	2.857%
22	15.656	2304	2307	2316	rVB	131155	196255	2.14%	0.354%
23	16.145	2385	2390	2405	rVB	123052	243058	2.65%	0.439%
24	16.715	2481	2487	2495	rBV	89168	180969	1.97%	0.327%
25	17.392	2596	2602	2610	rVB2	60528	142051	1.55%	0.256%
26	18.192	2734	2738	2749	rVB3	51353	136212	1.48%	0.246%

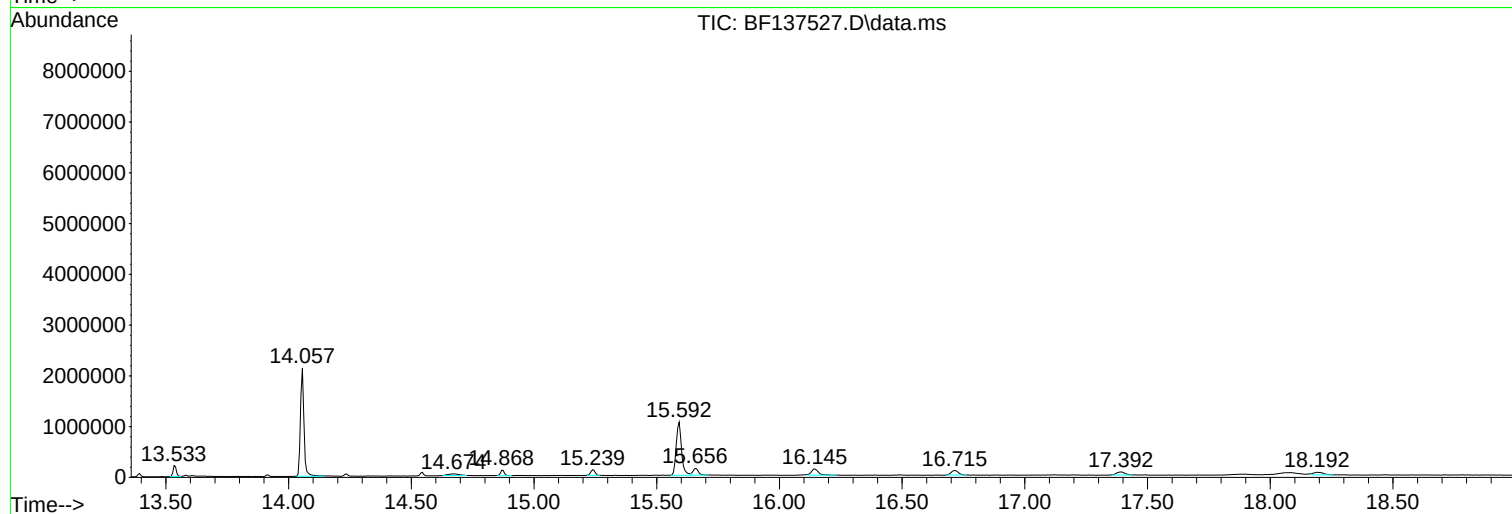
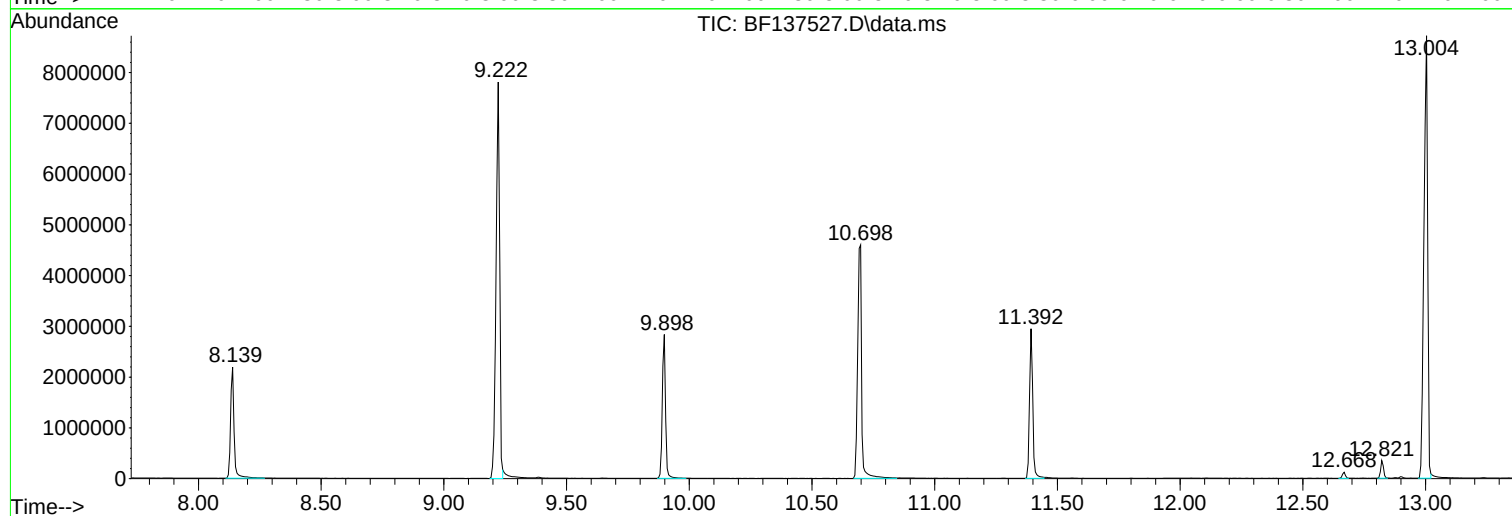
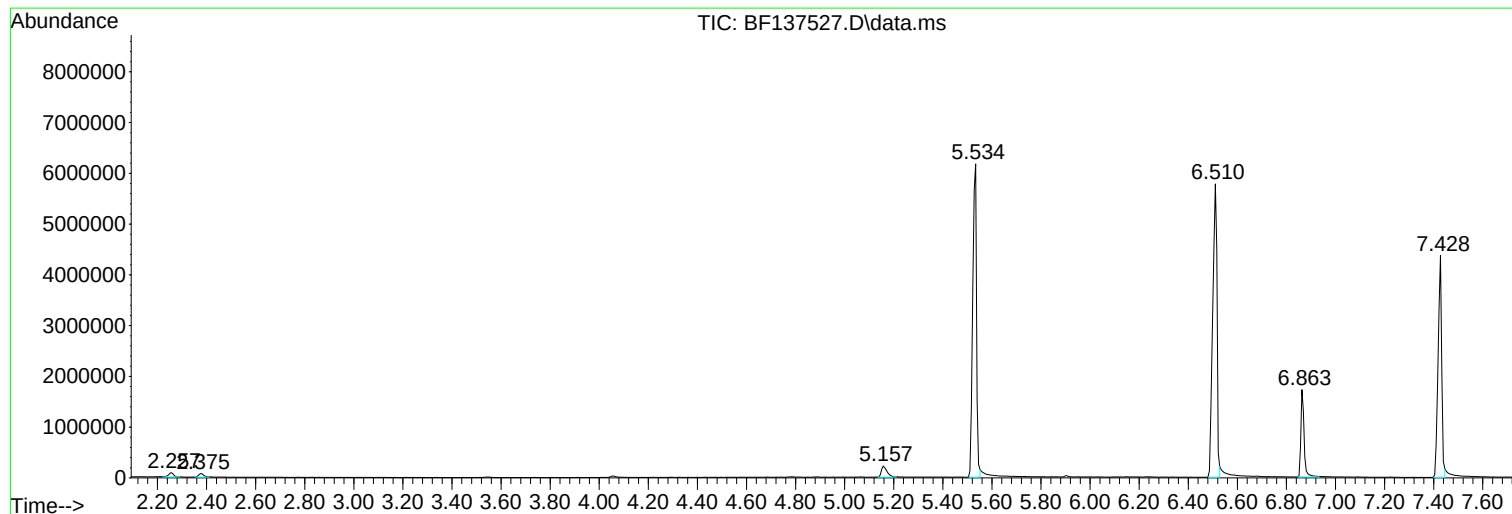
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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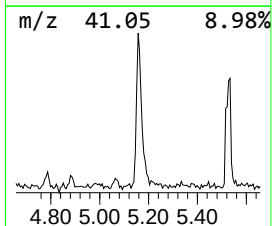
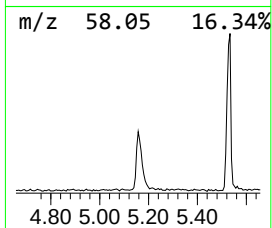
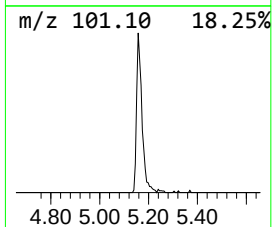
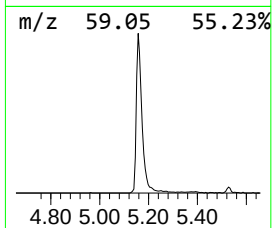
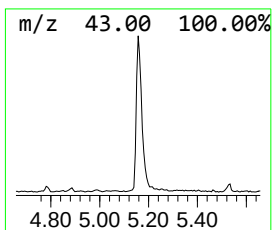
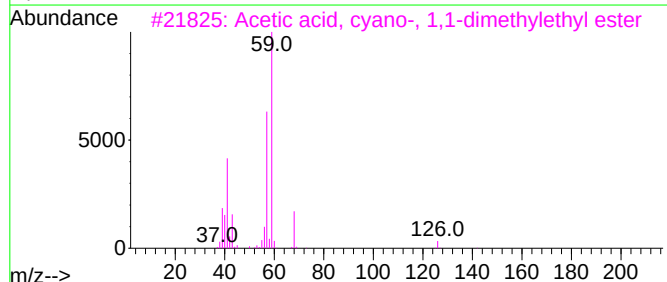
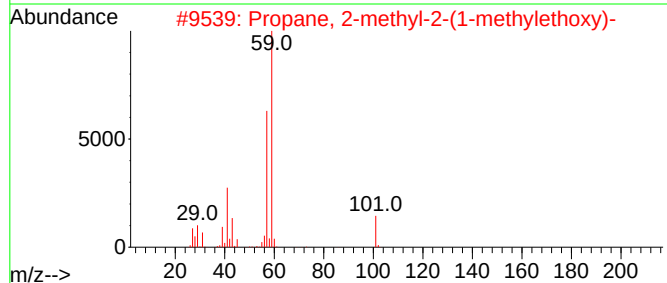
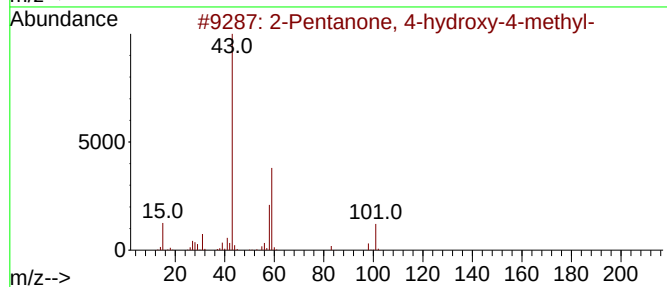
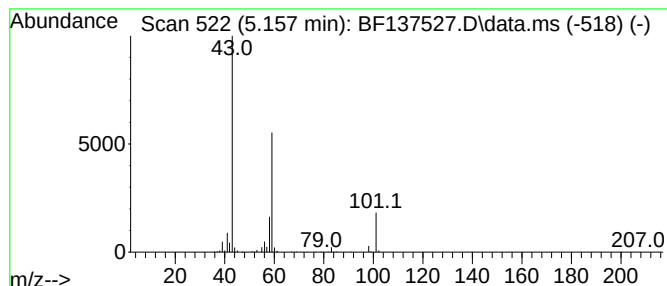
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
5.157	4.34 ng	335637	1,4-Dichlorobenzene-d4	6.863	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9



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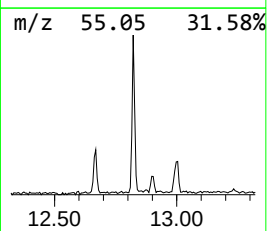
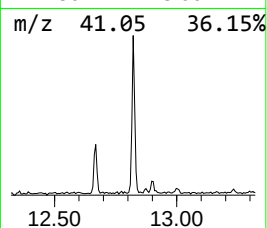
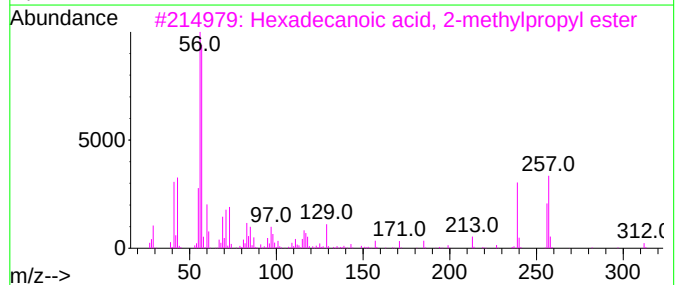
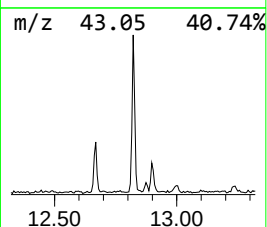
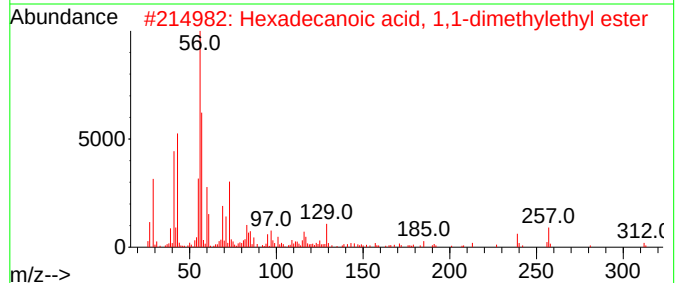
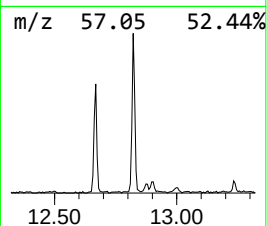
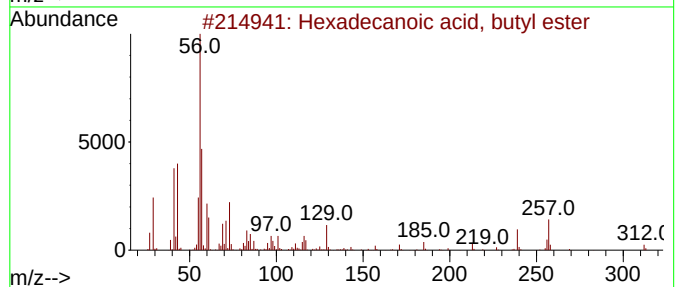
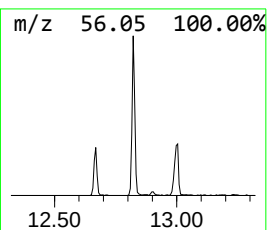
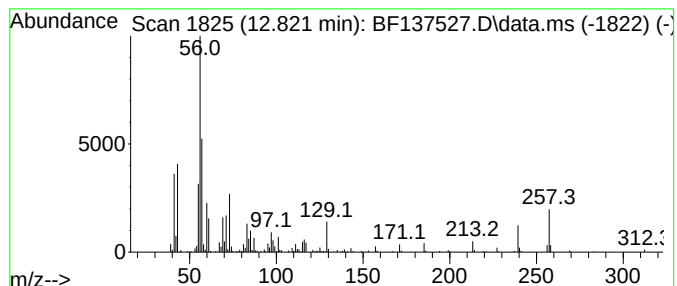
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.821	2.60 ng	276698	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	60
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	35



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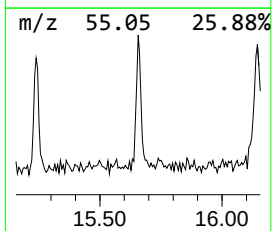
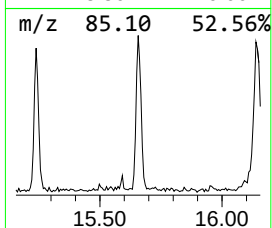
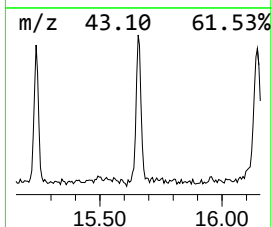
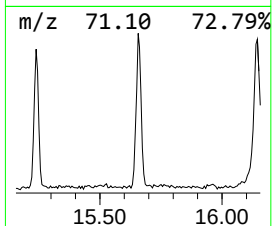
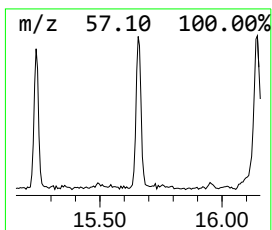
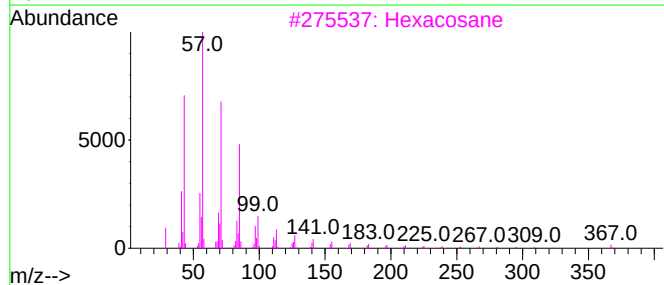
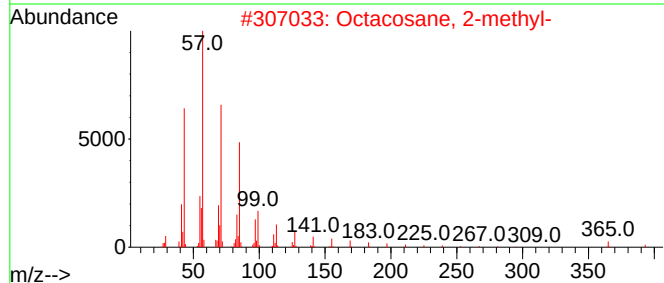
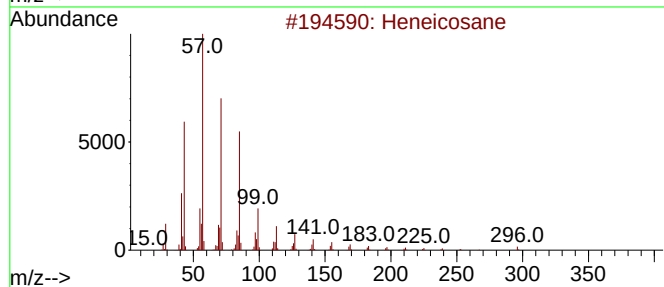
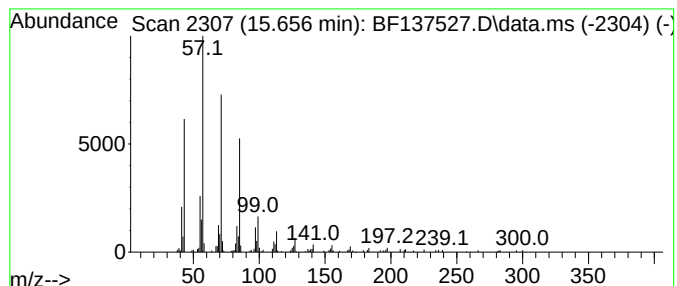
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.656	2.48 ng	196255	Perylene-d12	15.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Octadecane	254	C18H38	000593-45-3	87
5			Heptadecane	240	C17H36	000629-78-7	87



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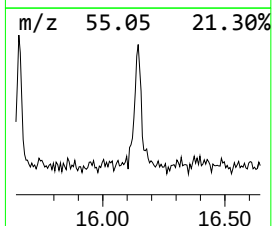
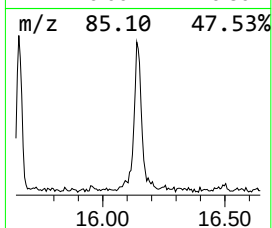
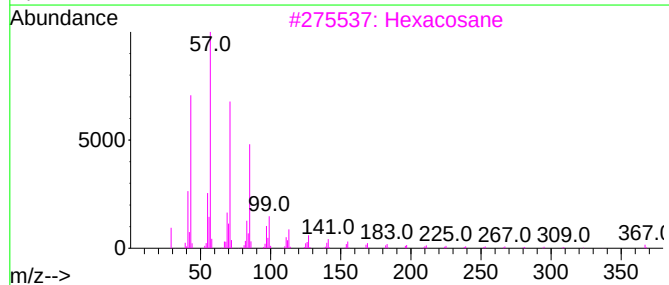
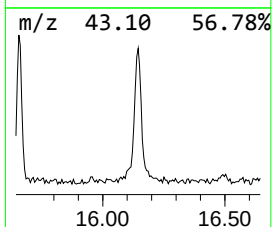
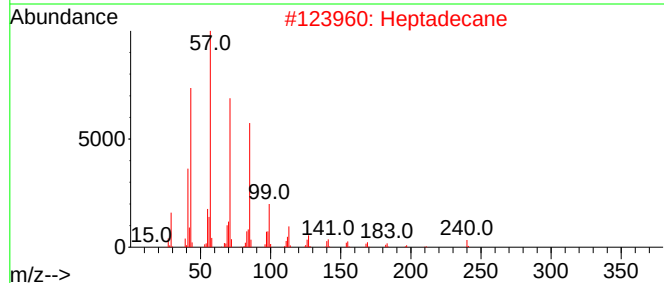
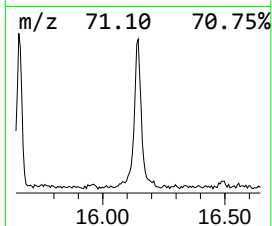
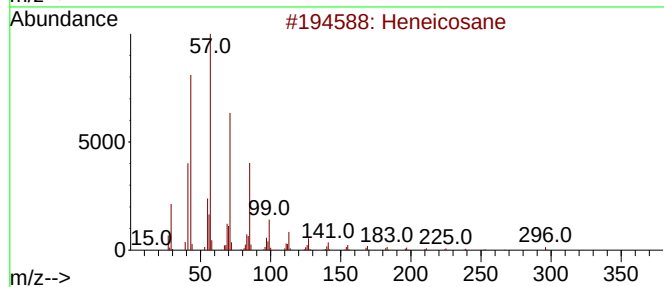
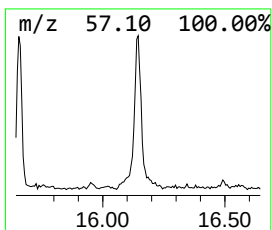
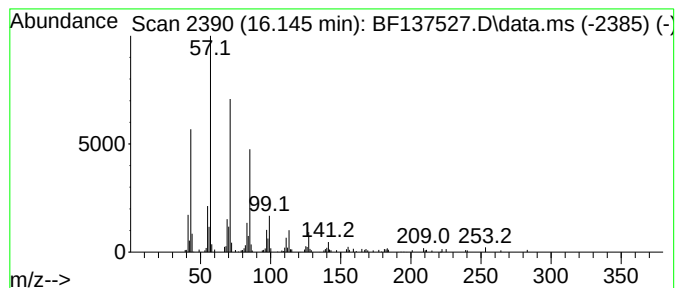
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Heptadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	3.07 ng	243058	Perylene-d12	15.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Heptadecane	240	C17H36	000629-78-7	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Hexatriacontane	507	C36H74	000630-06-8	91
5			Octacosane	394	C28H58	000630-02-4	91



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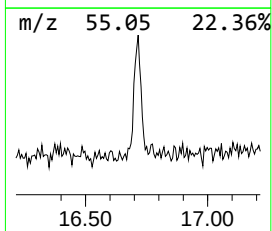
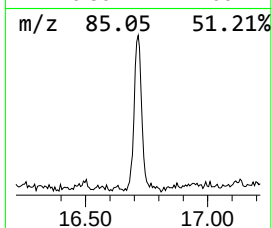
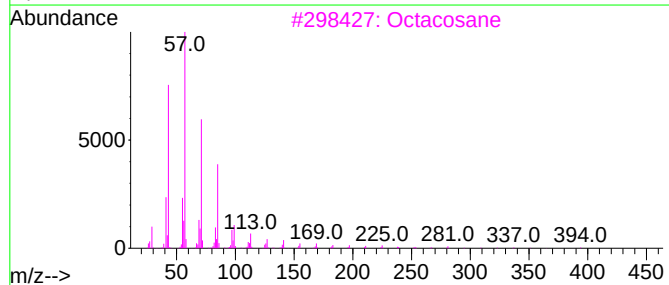
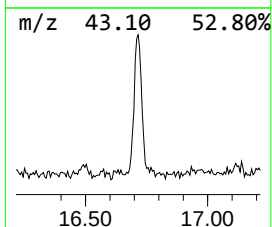
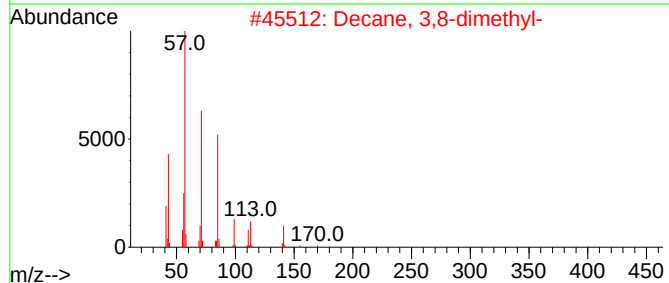
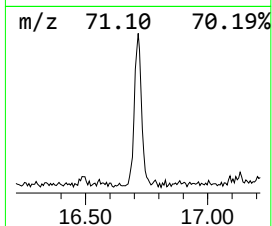
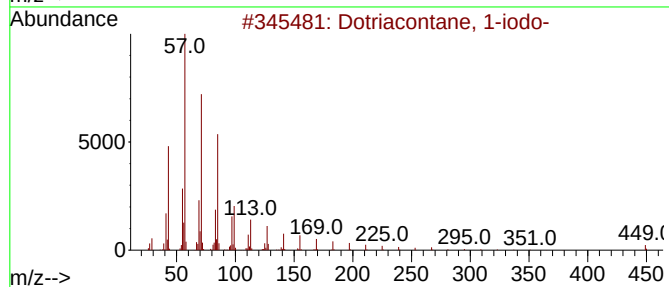
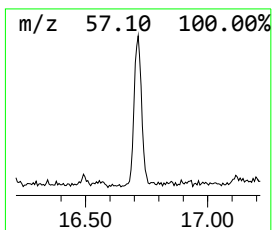
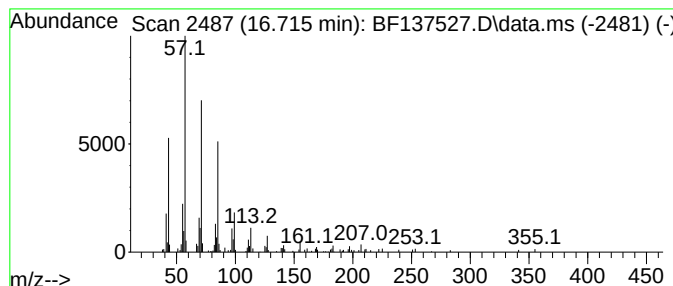
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dotriacontane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.715	2.29 ng	180969	Perylene-d12	15.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Nonadecane	268	C19H40	000629-92-5	87
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.157	4.3	ng	335637	1	6.863	1547790	20.0
Hexadecanoic ac...	12.821	2.6	ng	276698	5	14.057	2130200	20.0
Heneicosane	15.656	2.5	ng	196255	6	15.592	1582940	20.0
Heptadecane	16.145	3.1	ng	243058	6	15.592	1582940	20.0
Dotriacontane, ...	16.715	2.3	ng	180969	6	15.592	1582940	20.0