

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
 Data File : BF134874.D
 Acq On : 21 Aug 2023 18:43
 Operator : CG\JU
 Sample : 04070-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-1

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: BF134874.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	563	568	571	rBV	3245997	3171150	95.19%	12.792%
2	6.434	734	739	742	rBV	3163678	3198785	96.02%	12.903%
3	6.628	768	772	777	rBV2	134183	128587	3.86%	0.519%
4	6.793	796	800	806	rVB	1104541	898753	26.98%	3.625%
5	7.063	843	846	849	rVB	38400	36945	1.11%	0.149%
6	7.110	849	854	855	rBV2	37214	44669	1.34%	0.180%
7	7.181	862	866	870	rBV3	42308	49532	1.49%	0.200%
8	7.357	885	896	899	rBV	2134129	2138698	64.20%	8.627%
9	7.387	899	901	905	rVB	192405	142627	4.28%	0.575%
10	7.587	932	935	939	rVB	49017	52227	1.57%	0.211%
11	7.787	966	969	971	rBV2	36224	36688	1.10%	0.148%
12	7.863	980	982	985	rBV2	31317	34716	1.04%	0.140%
13	8.069	1011	1017	1020	rBV	1436934	1334733	40.06%	5.384%
14	8.363	1062	1067	1073	rVB5	38224	64696	1.94%	0.261%
15	8.451	1079	1082	1085	rVB3	51205	47904	1.44%	0.193%
16	8.492	1085	1089	1091	rBV	70841	64562	1.94%	0.260%
17	8.663	1114	1118	1121	rBV	289646	225020	6.75%	0.908%
18	8.781	1136	1138	1141	rVB	44416	35385	1.06%	0.143%
19	8.881	1152	1155	1159	rVB2	53405	53336	1.60%	0.215%
20	9.028	1176	1180	1183	rVB2	39438	41964	1.26%	0.169%
21	9.092	1189	1191	1196	rVB2	52440	45232	1.36%	0.182%
22	9.145	1196	1200	1204	rBV	3531749	3331520	100.00%	13.439%
23	9.228	1211	1214	1218	rBV	242274	197421	5.93%	0.796%
24	9.263	1218	1220	1224	rVB2	44607	42260	1.27%	0.170%
25	9.481	1254	1257	1260	rBV2	49415	46620	1.40%	0.188%
26	9.551	1264	1269	1271	rBV3	38442	46694	1.40%	0.188%
27	9.757	1302	1304	1309	rVB	131026	113763	3.41%	0.459%
28	9.828	1312	1316	1319	rVB	1278142	1139476	34.20%	4.596%
29	10.263	1387	1390	1392	rVB	88840	69629	2.09%	0.281%
30	10.481	1421	1427	1430	rBV2	24104	34126	1.02%	0.138%
31	10.616	1446	1450	1453	rBV	2135019	1783561	53.54%	7.195%
32	10.734	1468	1470	1477	rBV	62875	78693	2.36%	0.317%
33	11.316	1565	1569	1572	rBV	1099430	964256	28.94%	3.890%
34	11.851	1656	1660	1669	rBV	384605	379346	11.39%	1.530%
35	12.528	1771	1775	1779	rBV	28981	37620	1.13%	0.152%
36	12.639	1790	1794	1802	rBV	84708	115603	3.47%	0.466%

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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

37	12.910	1835	1840	1843	rBV	2862827	2487891	74.68%	10.036%
38	13.816	1990	1994	2001	rBV	214214	236750	7.11%	0.955%
39	13.963	2014	2019	2023	rBV	975632	909664	27.30%	3.669%
40	14.139	2046	2049	2052	rBV	86332	72516	2.18%	0.293%
41	14.445	2098	2101	2107	rBV2	55223	82144	2.47%	0.331%
42	14.827	2163	2166	2173	rVB	84542	94349	2.83%	0.381%
43	15.098	2209	2212	2217	rBV3	30981	39016	1.17%	0.157%
44	15.433	2264	2269	2275	rBV	506448	641255	19.25%	2.587%

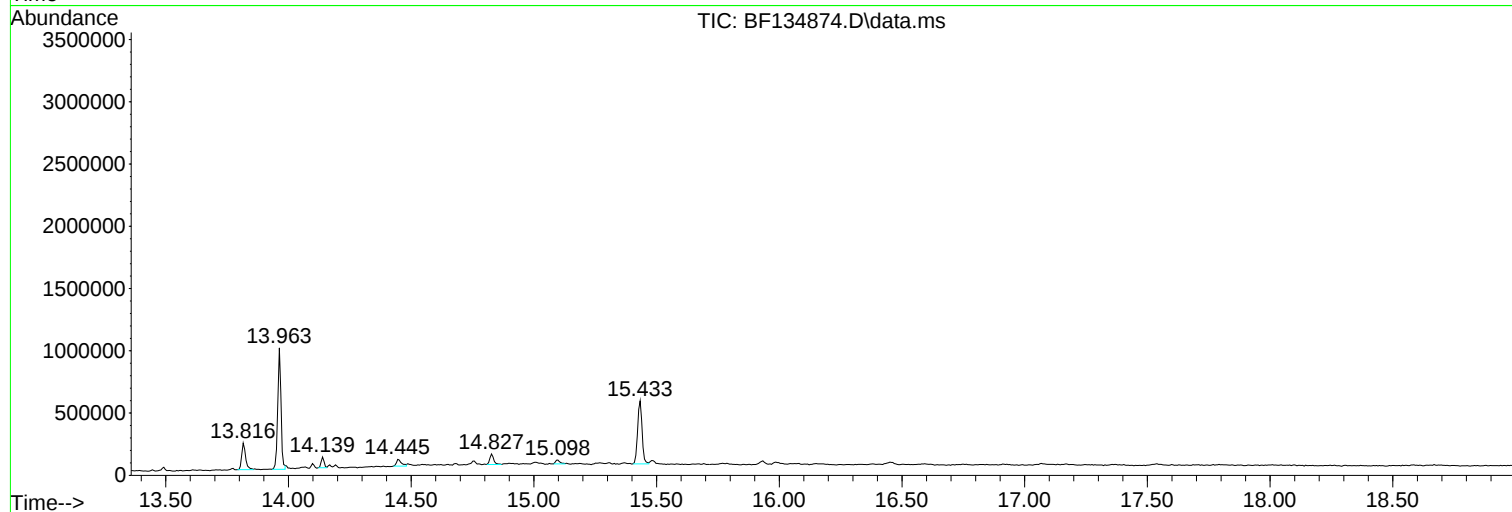
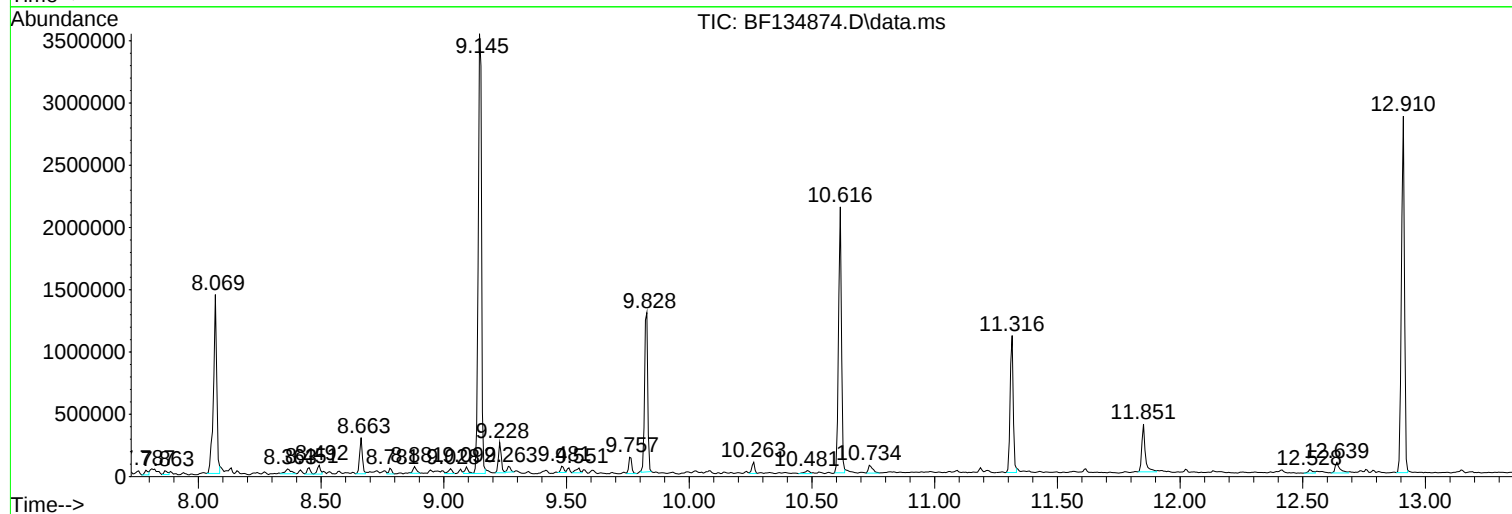
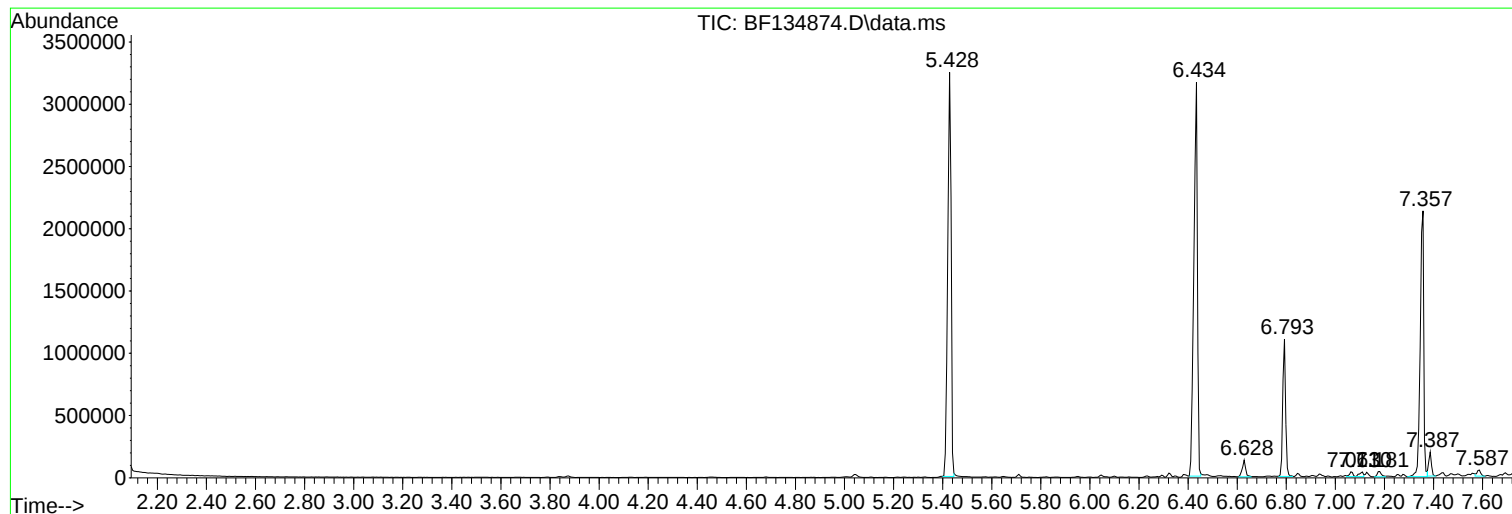
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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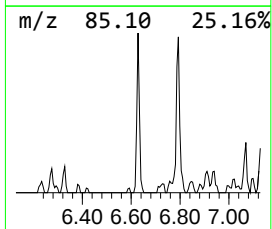
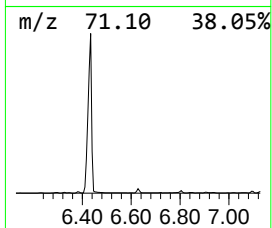
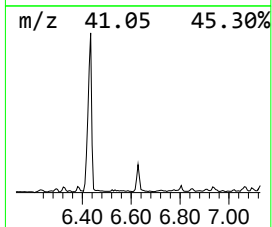
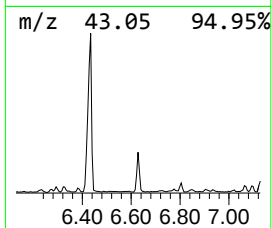
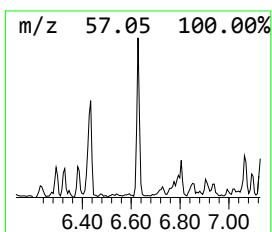
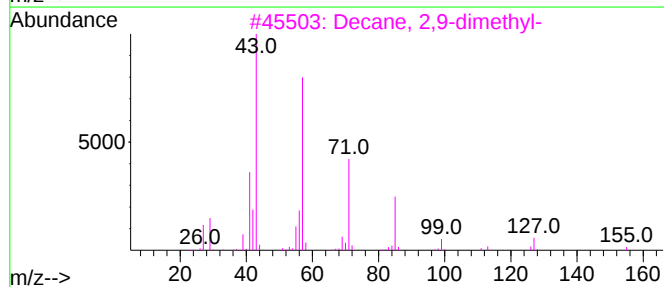
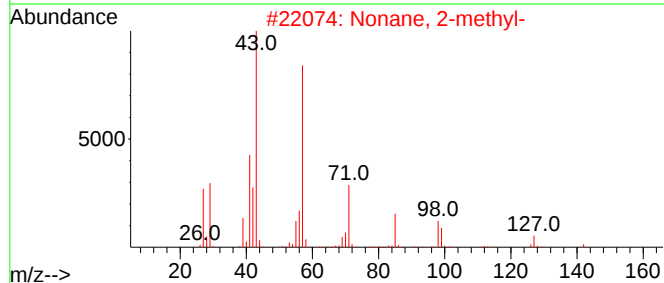
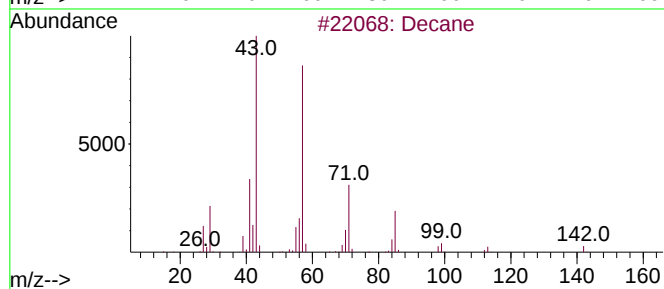
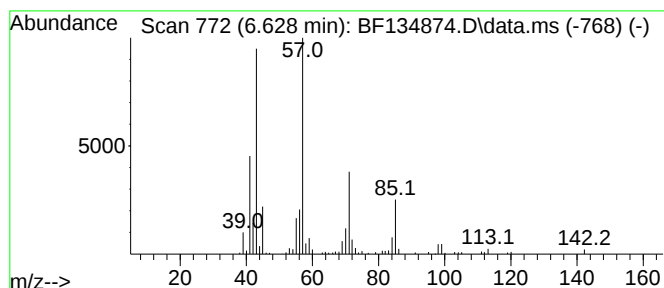
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Decane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.628	2.86 ng	128587	1,4-Dichlorobenzene-d4	6.793

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decane	142	C10H22	000124-18-5	72
2		Nonane, 2-methyl-	142	C10H22	000871-83-0	59
3		Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	53
4		Tridecane	184	C13H28	000629-50-5	53
5		Nonane	128	C9H20	000111-84-2	52



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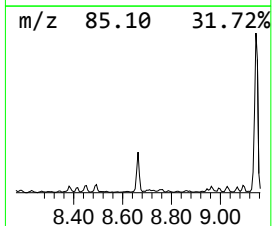
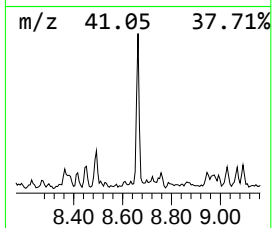
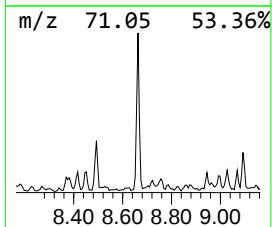
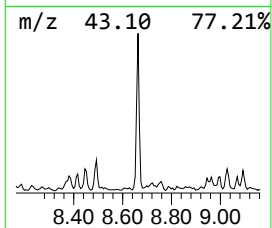
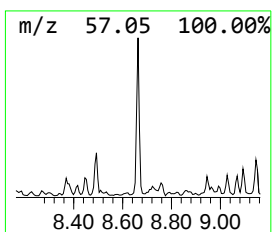
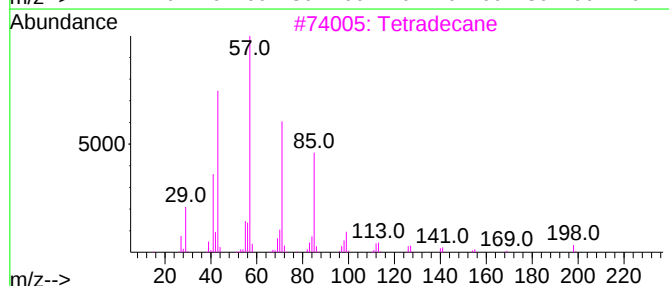
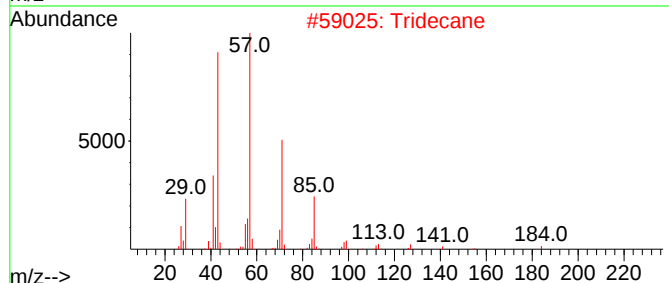
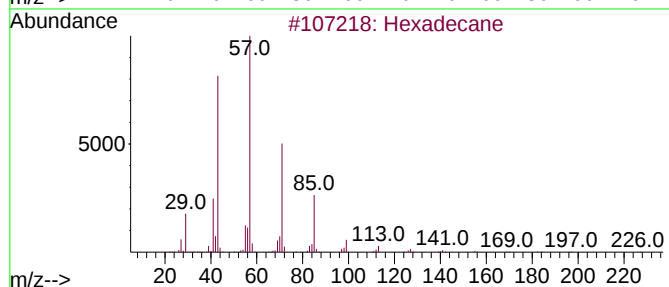
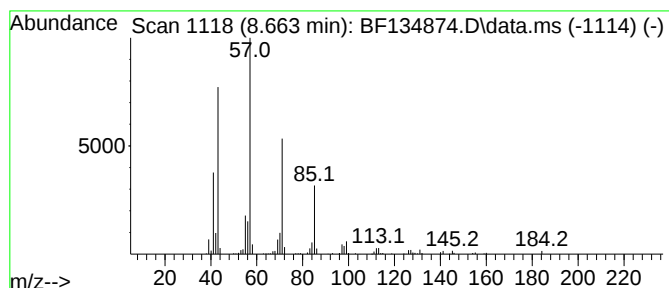
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.663	3.37 ng	225020	Naphthalene-d8	8.069

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	91
2		Tridecane	184	C13H28	000629-50-5	87
3		Tetradecane	198	C14H30	000629-59-4	86
4		Pentadecane	212	C15H32	000629-62-9	86
5		Tridecane, 7-propyl-	226	C16H34	055045-09-5	80



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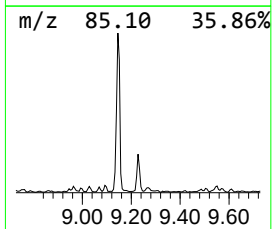
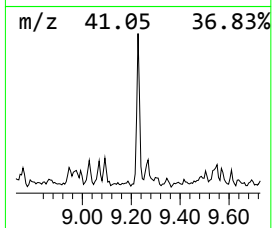
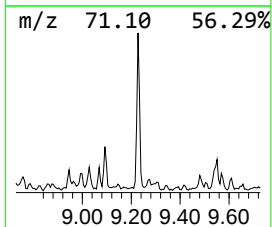
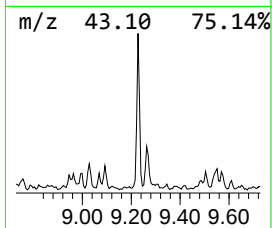
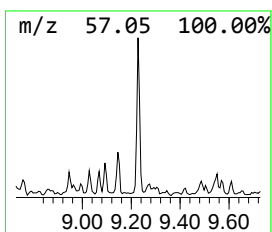
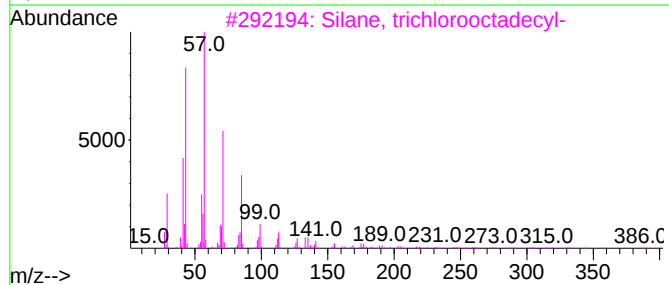
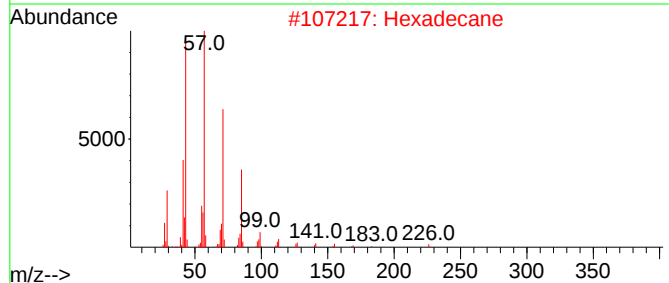
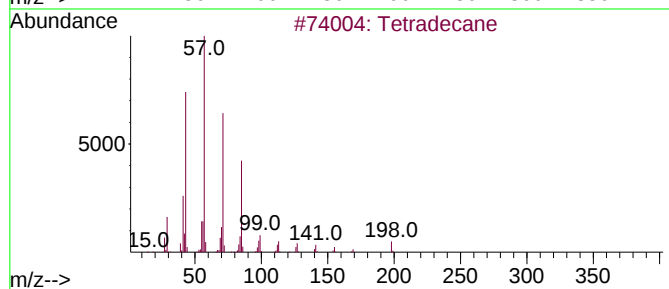
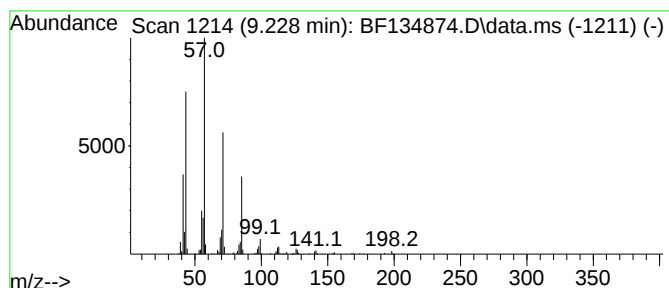
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.228	3.47 ng	197421	Acenaphthene-d10	9.828

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	94
2		Hexadecane	226	C16H34	000544-76-3	91
3		Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
4		Tridecane	184	C13H28	000629-50-5	86
5		Tridecane, 7-methyl-	198	C14H30	026730-14-3	76



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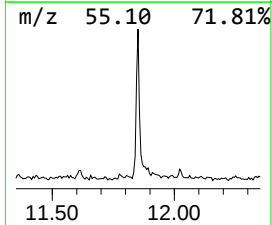
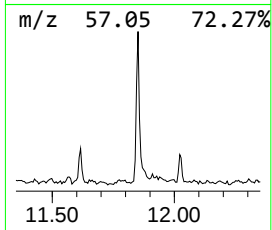
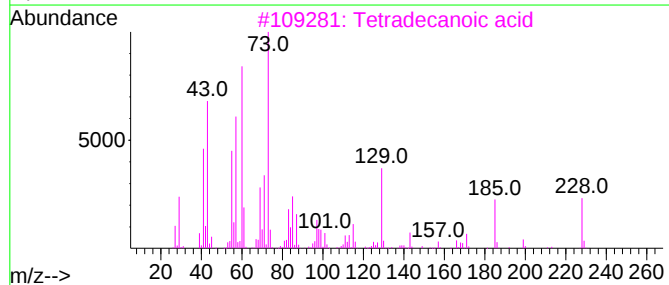
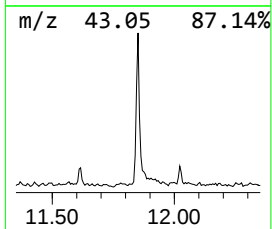
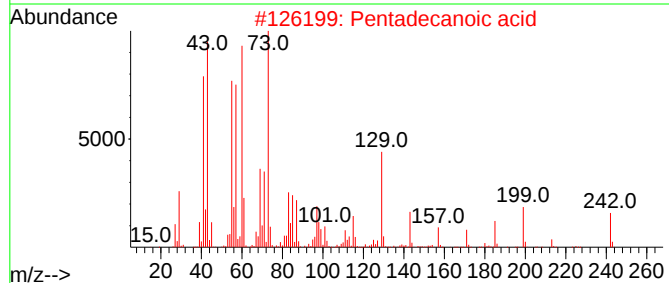
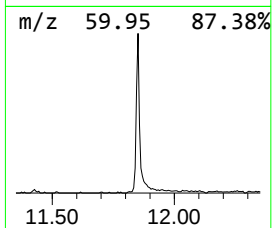
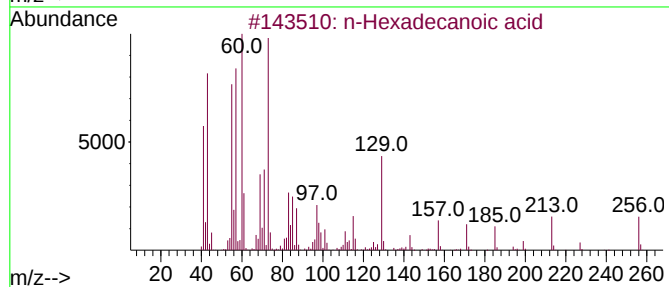
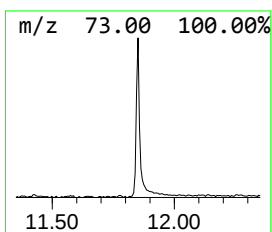
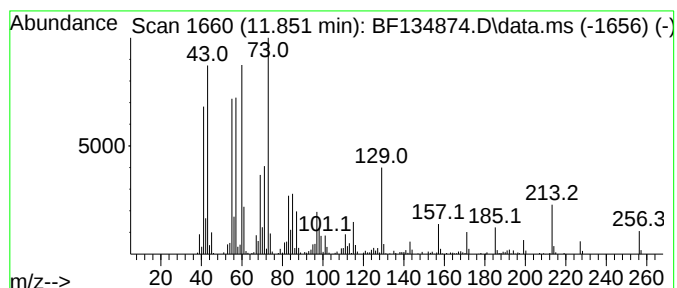
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.851	7.87 ng	379346	Phenanthrene-d10		11.316	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	91
4	Tridecanoic acid		214	C13H26O2	000638-53-9	91
5	n-Decanoic acid		172	C10H20O2	000334-48-5	76



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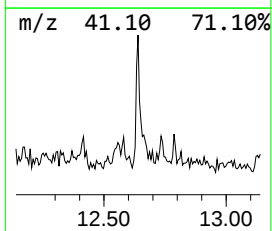
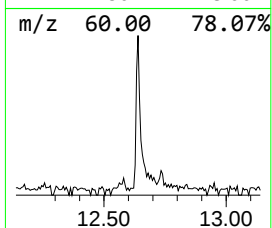
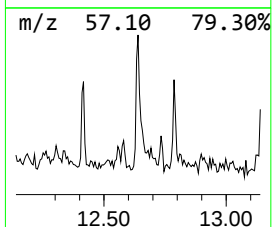
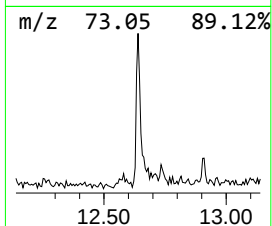
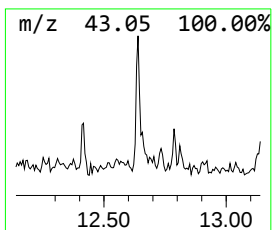
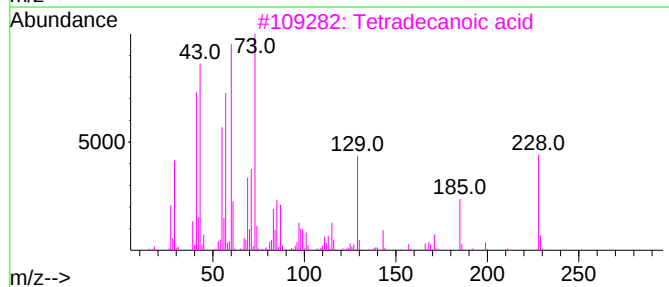
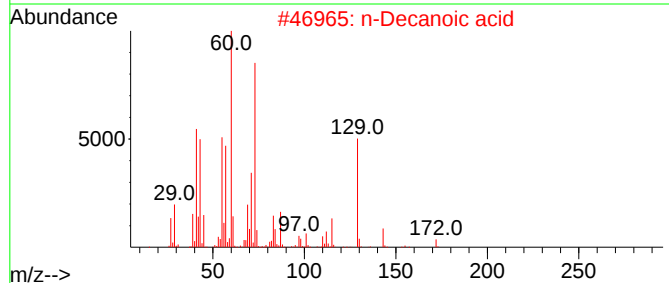
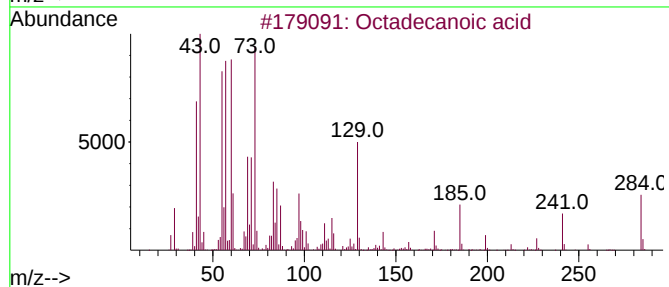
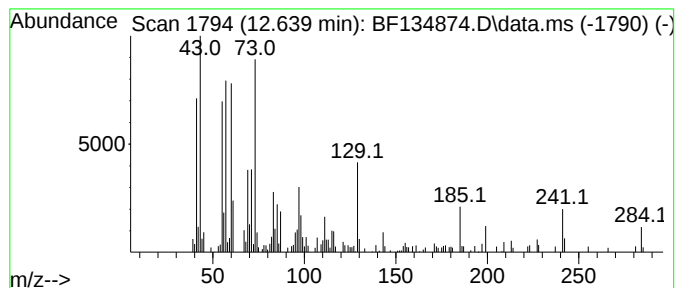
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	2.54 ng	115603	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	92
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
Data File : BF134874.D
Acq On : 21 Aug 2023 18:43
Operator : CG\JU
Sample : 04070-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

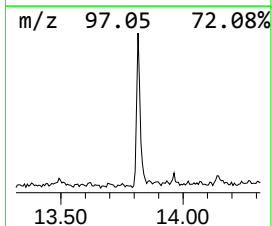
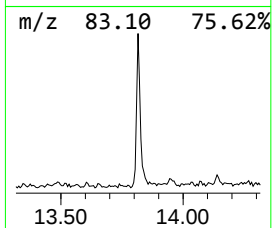
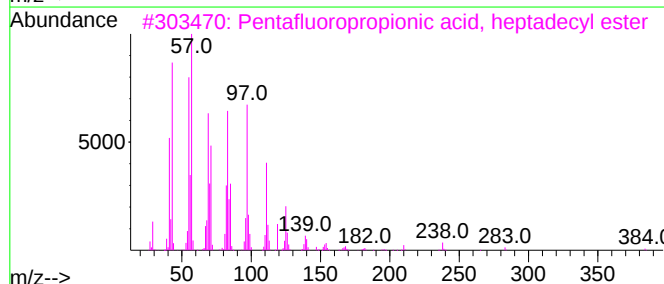
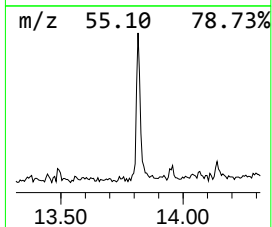
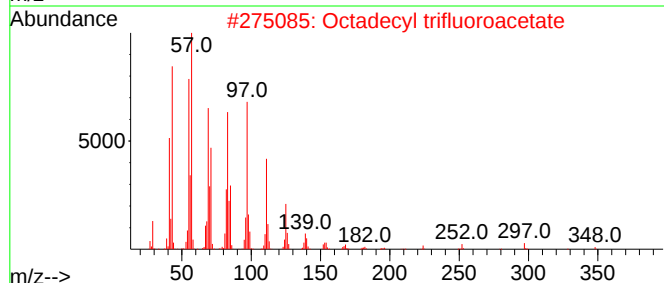
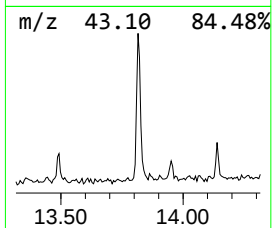
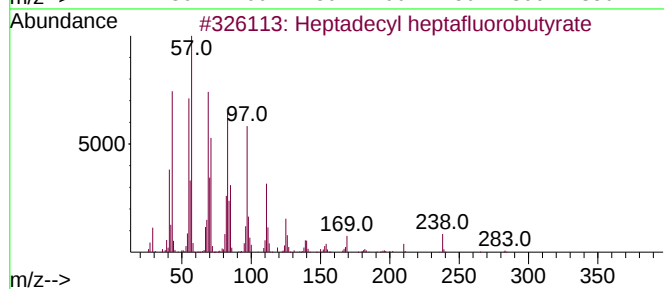
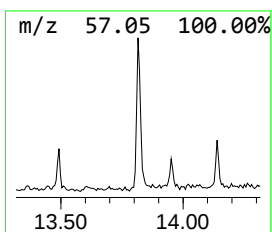
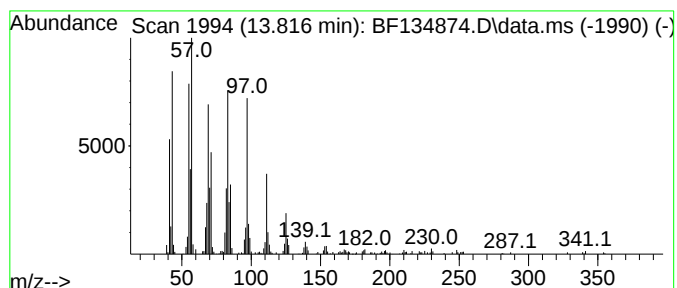
Instrument :
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ClientSampleId :
WC-1

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 6 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.816	5.21 ng	236750	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
Data File : BF134874.D
Acq On : 21 Aug 2023 18:43
Operator : CG\JU
Sample : 04070-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

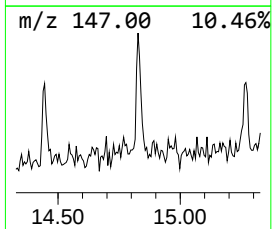
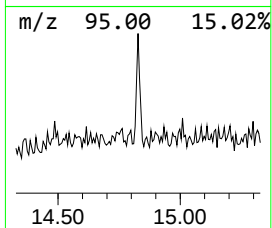
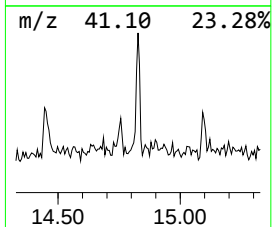
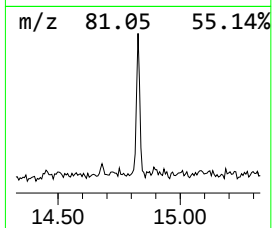
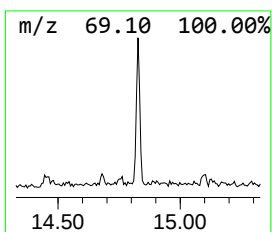
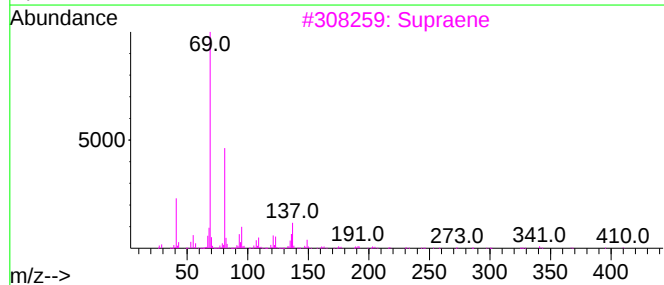
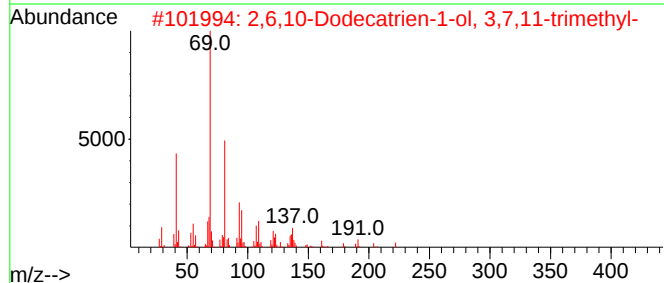
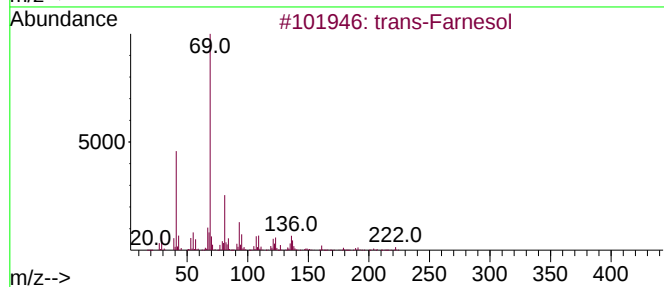
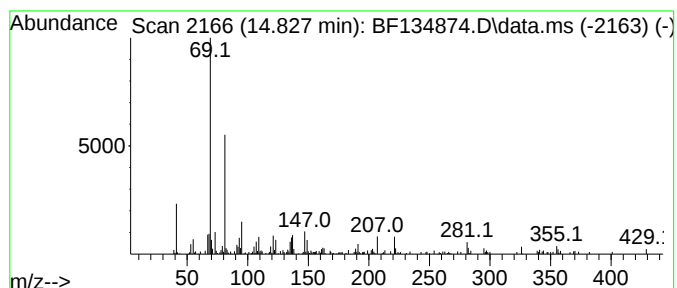
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 trans-Farnesol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.827	2.94 ng	94349	Perylene-d12	15.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Farnesol	222	C15H26O	000106-28-5	64
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	62
3	Supraene	410	C30H50	007683-64-9	58
4	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	58
5	Fumaric acid, 8-chlorooctyl trid...	444	C25H45ClO4	1000348-53-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082123\
Data File : BF134874.D
Acq On : 21 Aug 2023 18:43
Operator : CG\JU
Sample : 04070-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Decane	6.628	2.9	ng	128587	1	6.793	898753	20.0
Hexadecane	8.663	3.4	ng	225020	2	8.069	1334730	20.0
Tetradecane	9.228	3.5	ng	197421	3	9.828	1139480	20.0
n-Hexadecanoic ...	11.851	7.9	ng	379346	4	11.316	964256	20.0
Octadecanoic acid	12.639	2.5	ng	115603	5	13.963	909664	20.0
Heptadecyl hept...	13.816	5.2	ng	236750	5	13.963	909664	20.0
trans-Farnesol	14.827	2.9	ng	94349	6	15.433	641255	20.0