

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
 Data File : BF135608.D
 Acq On : 05 Oct 2023 19:43
 Operator : CG\JU
 Sample : 04712-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-2

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	484	489	510	rBV	946841	1252279	42.75%	5.639%
2	5.375	556	559	576	rBV	2829839	2890678	98.69%	13.016%
3	5.757	621	624	629	rBV	31435	30629	1.05%	0.138%
4	6.387	728	731	748	rBV	2697969	2929056	100.00%	13.188%
5	6.581	761	764	776	rBV	51094	74306	2.54%	0.335%
6	6.739	787	791	801	rBV	1003625	897913	30.66%	4.043%
7	7.281	879	883	884	rBV	257881	203605	6.95%	0.917%
8	7.304	884	887	890	rVB	2085416	1693385	57.81%	7.625%
9	8.016	1004	1008	1024	rBV	1432265	1188042	40.56%	5.349%
10	9.092	1187	1191	1195	rBV	3012550	2687857	91.77%	12.102%
11	9.210	1208	1211	1220	rVB	163910	159576	5.45%	0.719%
12	9.775	1303	1307	1310	rBV	1277279	1157515	39.52%	5.212%
13	10.569	1438	1442	1455	rBV	1658895	1489937	50.87%	6.709%
14	11.269	1557	1561	1564	rBV	1087112	1003866	34.27%	4.520%
15	11.292	1564	1565	1568	rVB	64394	35564	1.21%	0.160%
16	11.804	1649	1652	1663	rBV2	232506	294336	10.05%	1.325%
17	12.368	1742	1748	1754	rVB6	25609	37028	1.26%	0.167%
18	12.486	1765	1768	1772	rBV	94396	95275	3.25%	0.429%
19	12.592	1783	1786	1792	rBV	106050	141240	4.82%	0.636%
20	12.721	1802	1808	1812	rVB	73672	93326	3.19%	0.420%
21	12.863	1828	1832	1835	rBV	1972987	1731269	59.11%	7.795%
22	13.439	1926	1930	1932	rBV2	36568	38948	1.33%	0.175%
23	13.768	1983	1986	1988	rBV	46321	49334	1.68%	0.222%
24	13.804	1988	1992	2001	rVB9	40851	116636	3.98%	0.525%
25	13.927	2009	2013	2016	rBV	835855	789410	26.95%	3.554%
26	14.086	2037	2040	2043	rBV	48699	52472	1.79%	0.236%
27	14.392	2090	2092	2095	rVB	46619	38713	1.32%	0.174%
28	14.698	2141	2144	2147	rVB	44217	39837	1.36%	0.179%
29	14.968	2188	2190	2197	rBV	34829	67942	2.32%	0.306%
30	15.027	2197	2200	2204	rVB	69811	87167	2.98%	0.392%
31	15.392	2258	2262	2272	rVB	646354	842167	28.75%	3.792%

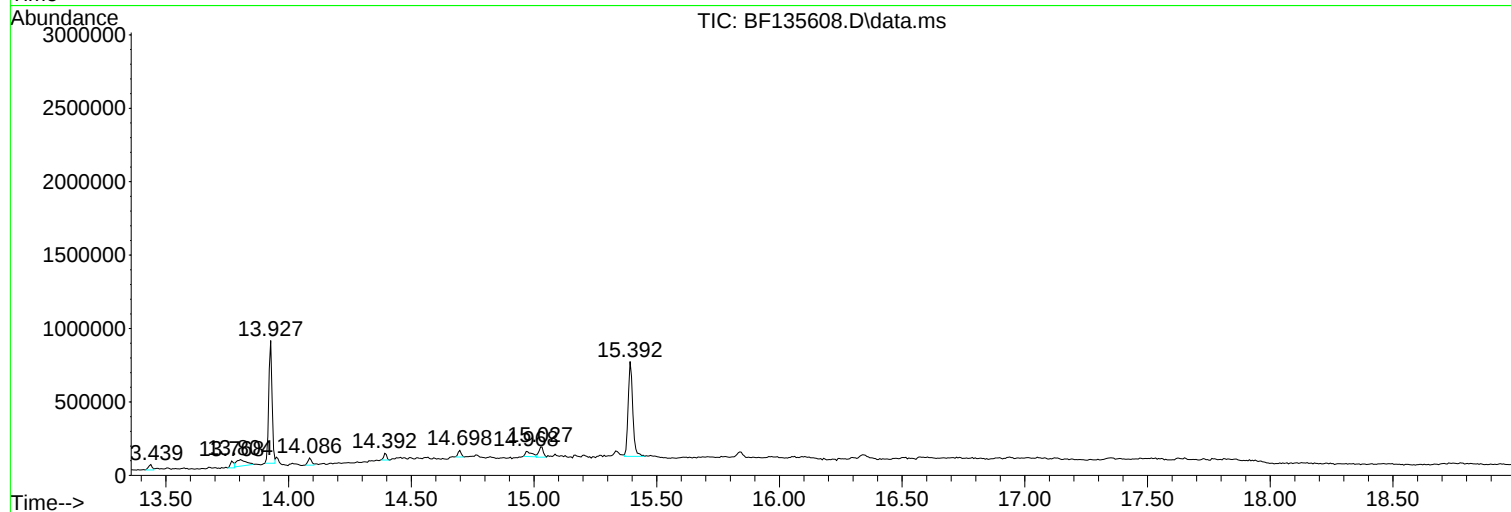
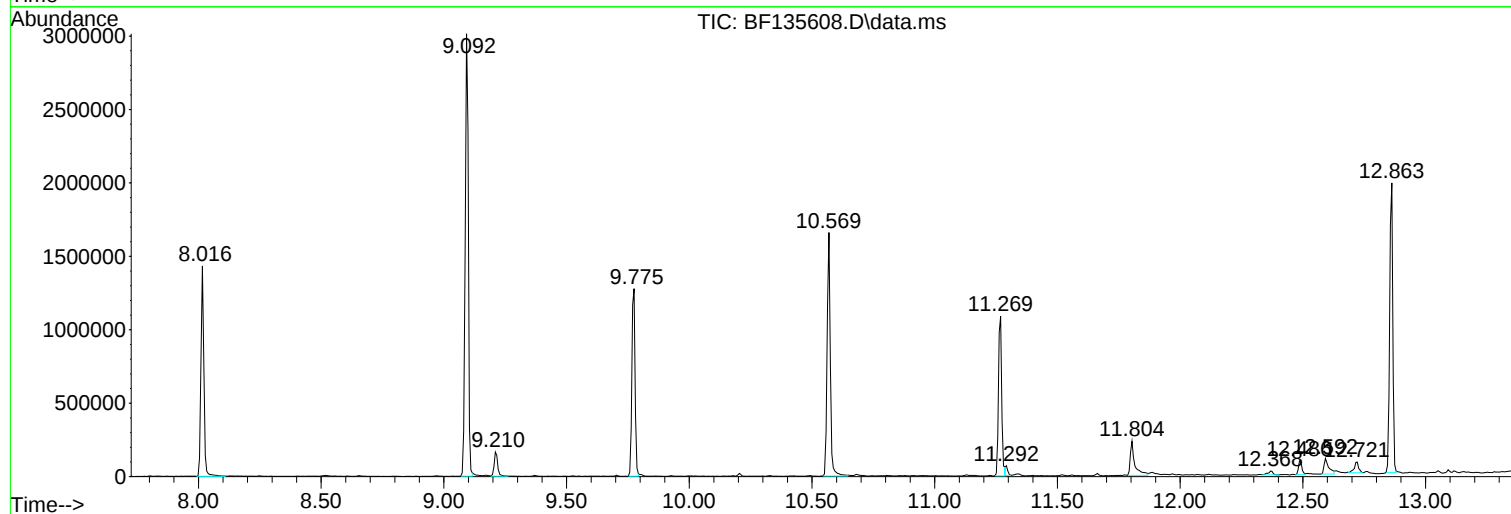
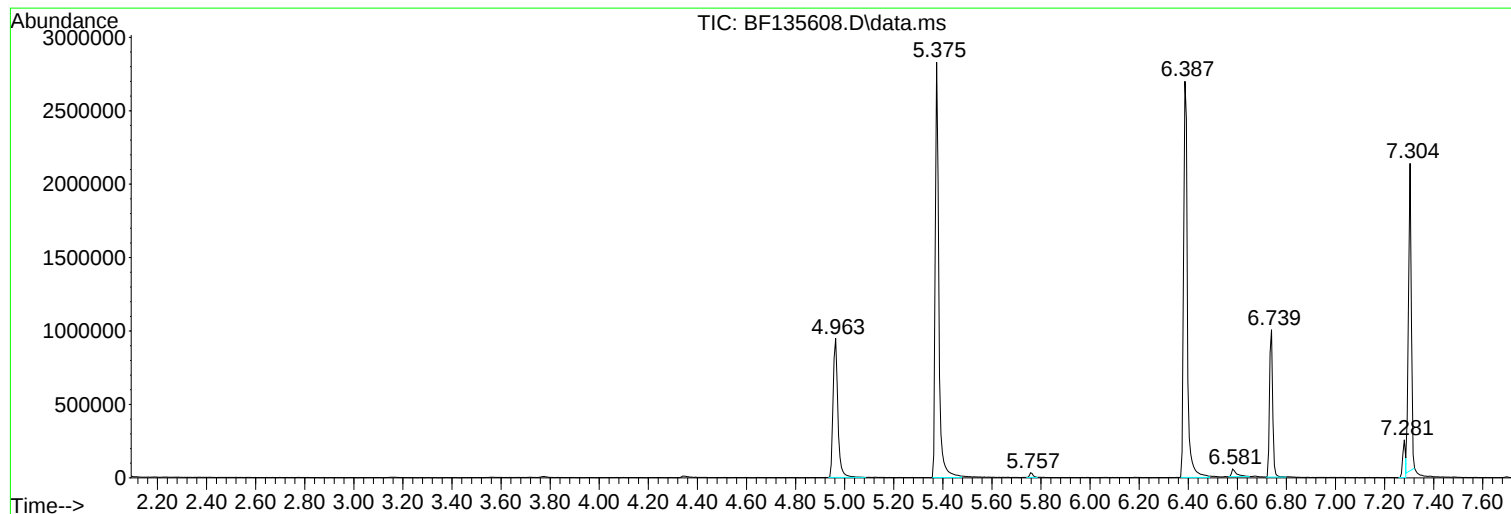
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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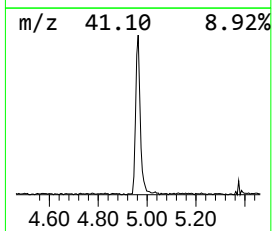
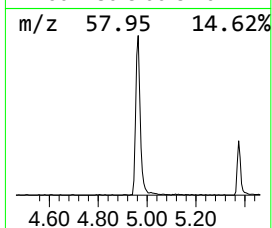
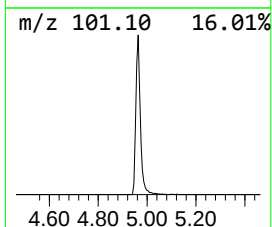
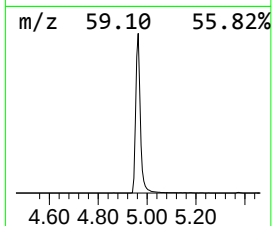
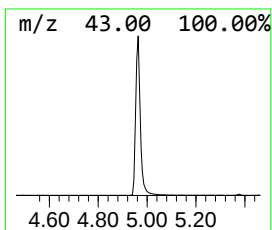
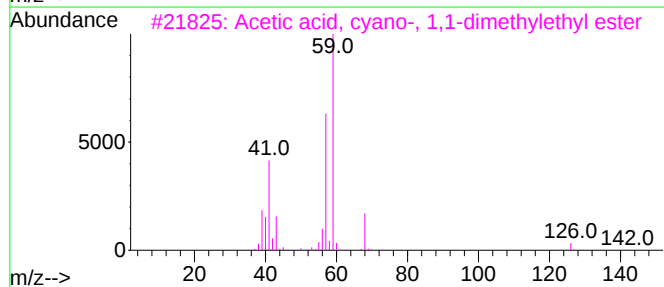
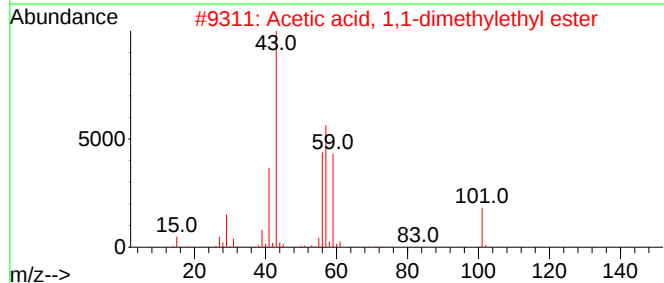
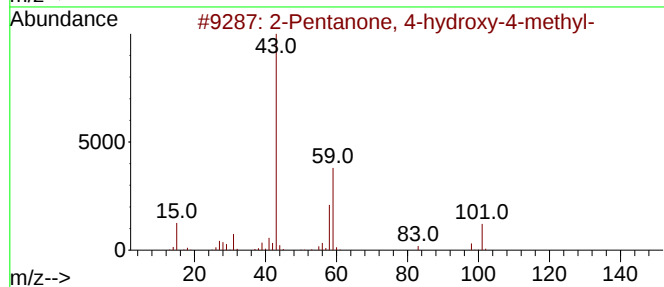
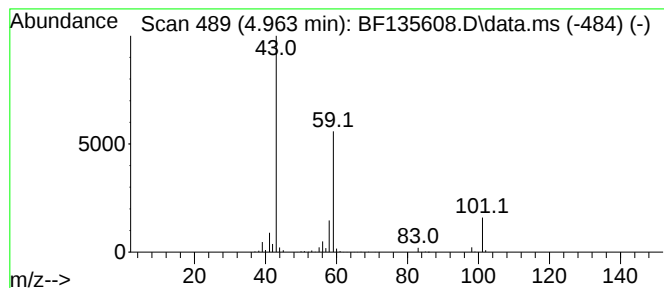
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	27.89 ng	1252280	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
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	25		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9		
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9		



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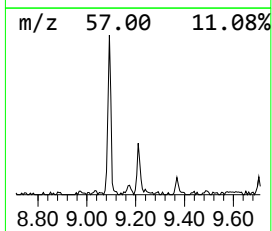
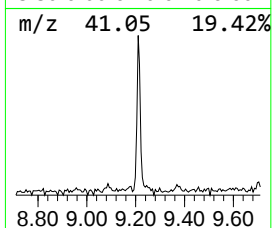
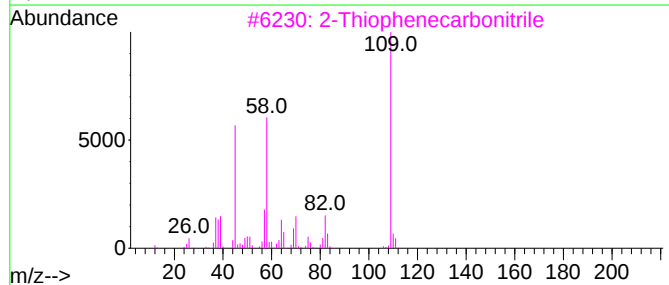
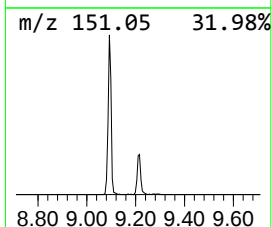
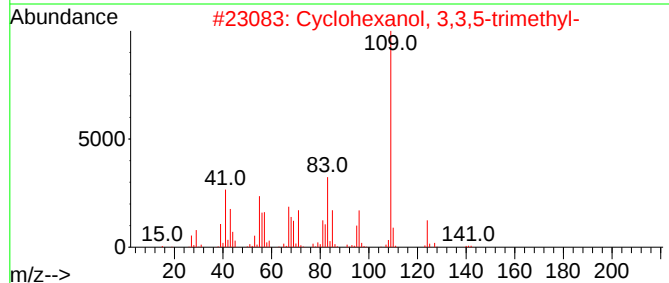
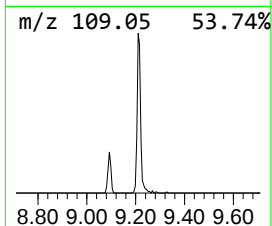
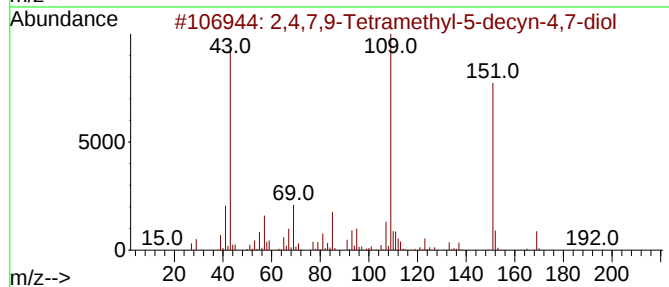
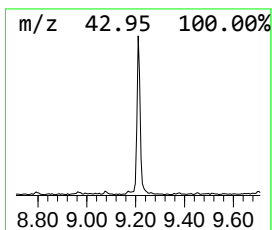
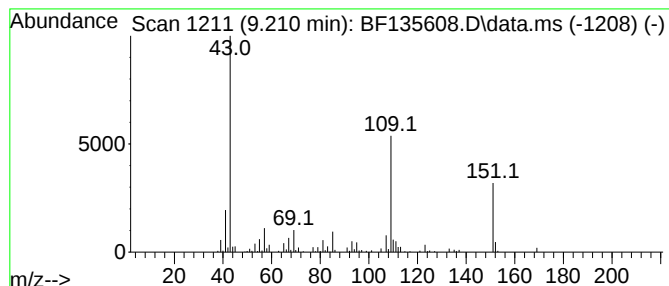
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.210	2.76 ng	159576	Acenaphthene-d10	9.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	86	
2	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	50	
3	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	47	
4	Metacetamol	151	C8H9NO2	000621-42-1	47	
5	Acetaminophen	151	C8H9NO2	000103-90-2	43	



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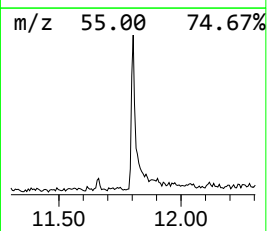
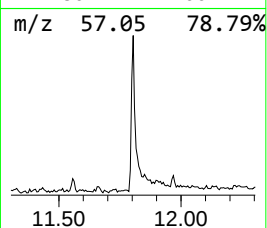
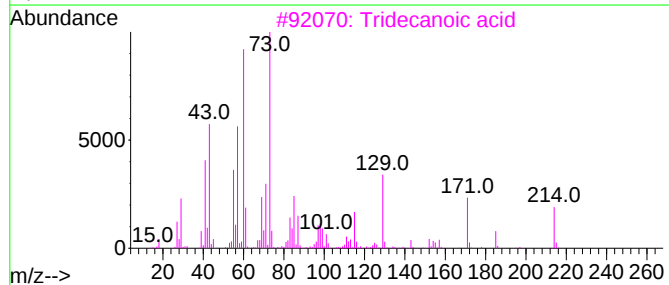
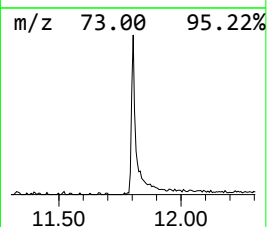
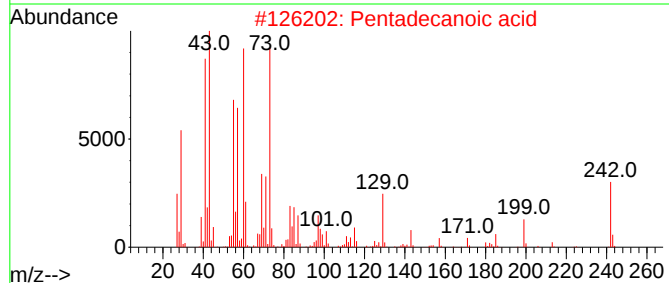
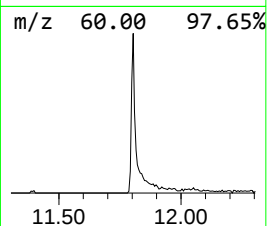
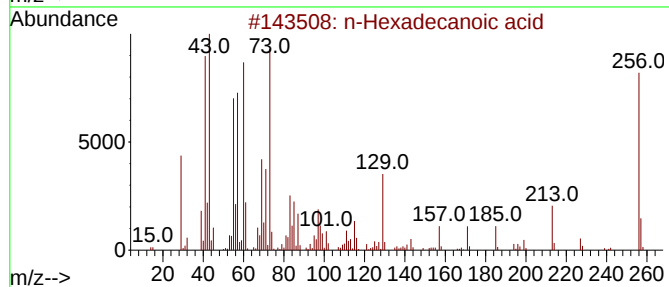
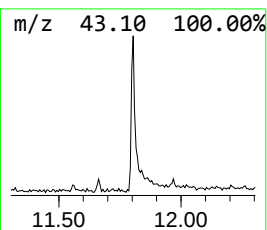
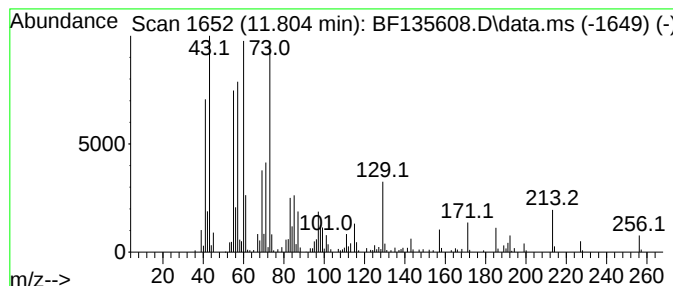
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	5.86 ng	294336	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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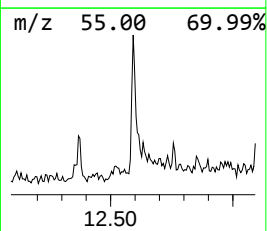
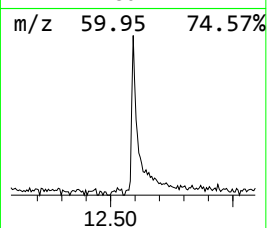
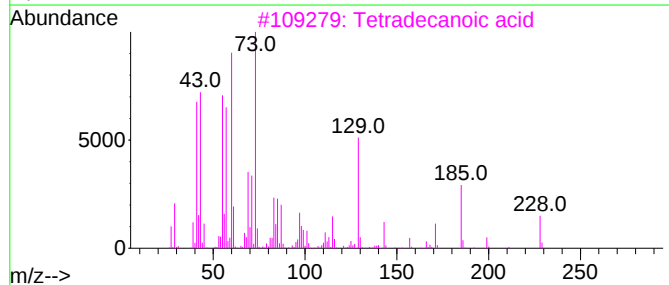
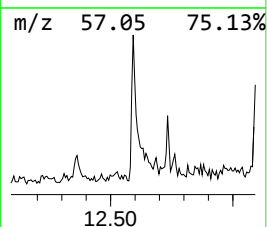
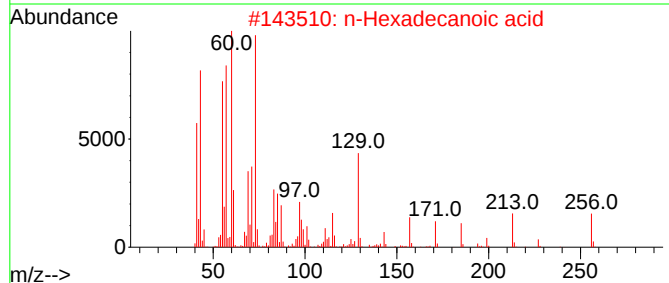
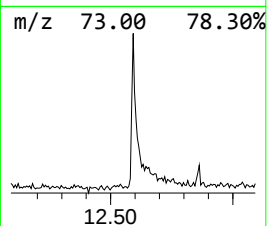
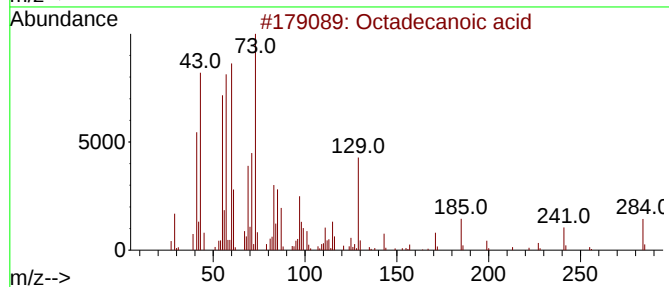
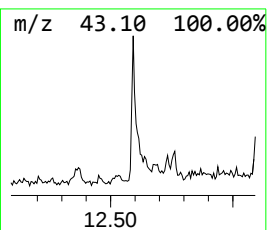
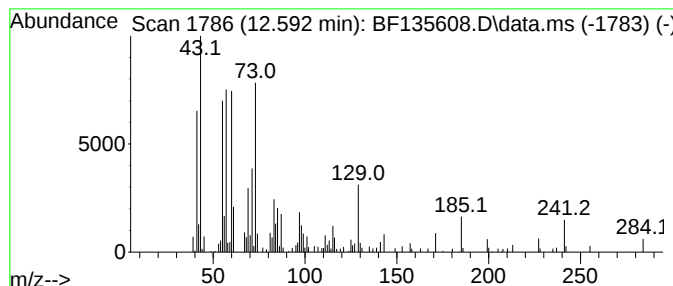
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	2.81 ng	141240	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Undecanoic acid	186	C11H22O2	000112-37-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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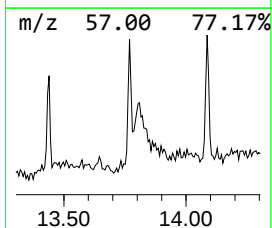
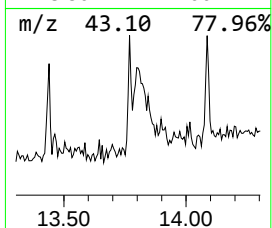
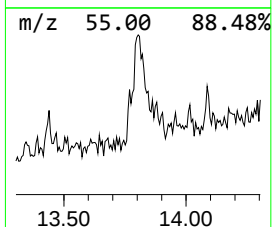
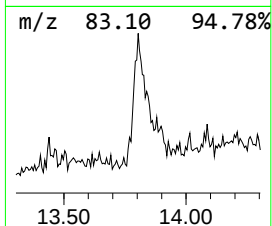
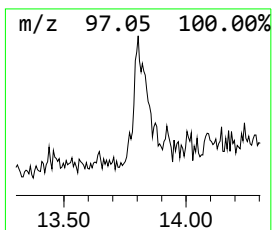
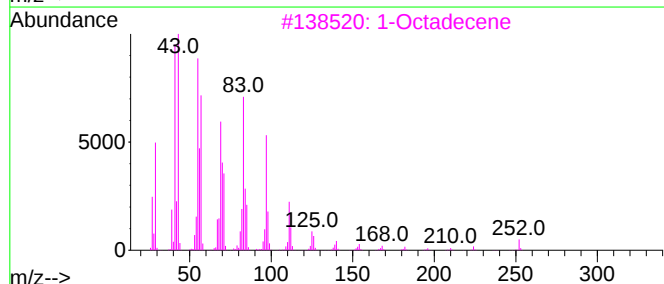
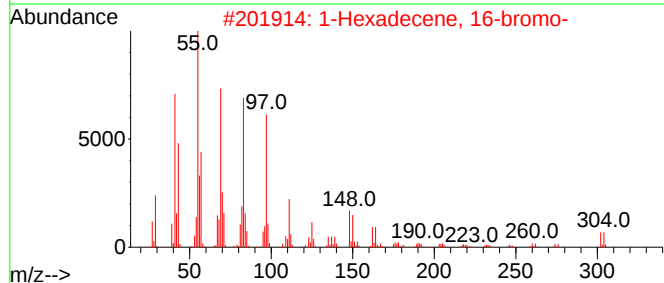
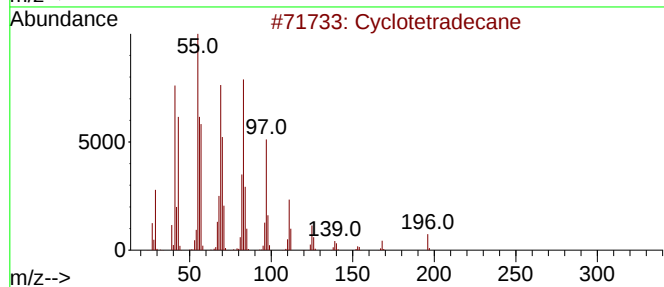
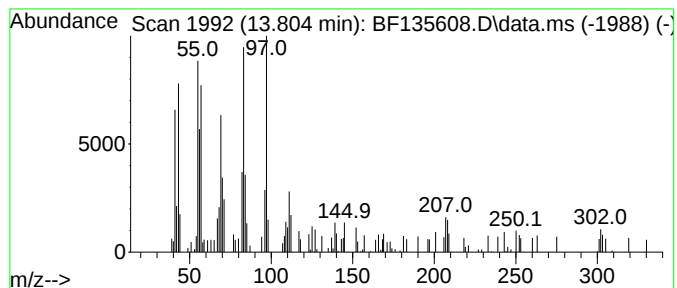
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Peak Number 6 Cyclotetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	2.96 ng	116636	Chrysene-d12	13.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	93
2			1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	80
3			1-Octadecene	252	C18H36	000112-88-9	64
4			1-Tetradecene	196	C14H28	001120-36-1	50
5			Cyclohexadecane	224	C16H32	000295-65-8	49



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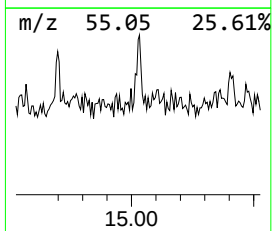
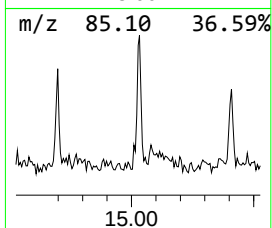
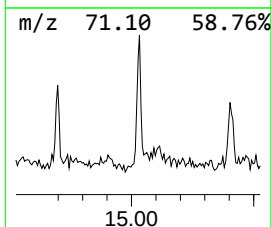
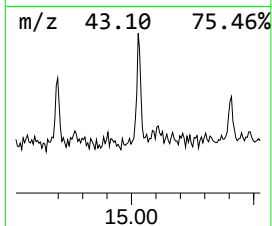
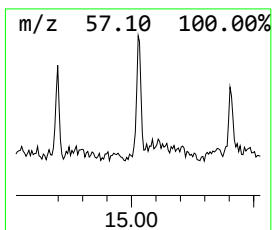
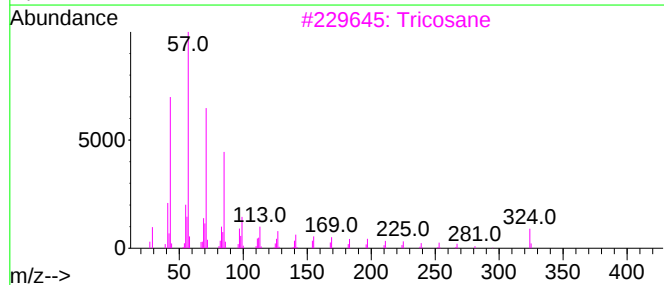
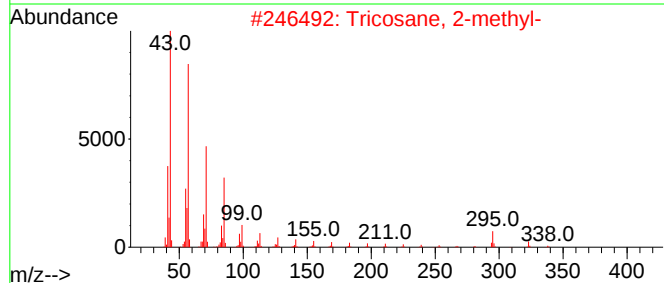
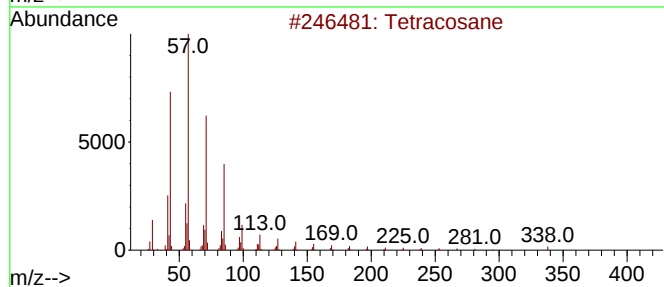
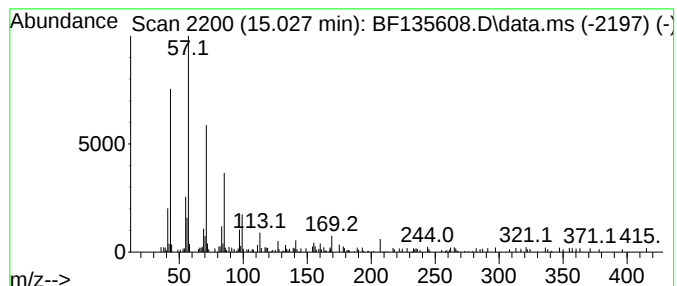
Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.027	2.07 ng	87167	Perylene-d12	15.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87
3	Tricosane	324	C23H48	000638-67-5	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
Data File : BF135608.D
Acq On : 05 Oct 2023 19:43
Operator : CG\JU
Sample : 04712-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
unknown-01	4.963	27.9	ng	1252280	1	6.739	897913	20.0
2,4,7,9-Tetrame...	9.210	2.8	ng	159576	3	9.775	1157520	20.0
n-Hexadecanoic ...	11.804	5.9	ng	294336	4	11.269	1003870	20.0
Octadecanoic acid	12.592	2.8	ng	141240	4	11.269	1003870	20.0
Cyclotetradecane	13.804	3.0	ng	116636	5	13.927	789410	20.0
Tetracosane	15.027	2.1	ng	87167	6	15.392	842167	20.0