

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011323\
 Data File : BF132057.D
 Acq On : 13 Jan 2023 13:50
 Operator : CG\JU
 Sample : PB150221BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB150221BL

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-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132057.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	18	rVB	34312	46806	1.17%	0.215%
2	4.998	488	495	505	rBV	64794	105286	2.63%	0.484%
3	5.404	559	564	576	rBV	2587183	2606816	65.06%	11.976%
4	6.428	733	738	741	rBV	2538204	2568428	64.11%	11.800%
5	6.775	793	797	800	rBV	582649	504528	12.59%	2.318%
6	7.351	889	895	898	rBV	1567554	1721809	42.97%	7.910%
7	8.063	1011	1016	1020	rBV	717257	650283	16.23%	2.987%
8	9.145	1194	1200	1203	rBV	3343761	3356013	83.76%	15.418%
9	9.822	1310	1315	1319	rBV	924424	800986	19.99%	3.680%
10	10.622	1446	1451	1454	rBV	2436955	2218385	55.37%	10.192%
11	11.316	1563	1569	1572	rBV	1116536	889194	22.19%	4.085%
12	11.663	1624	1628	1633	rBV	100648	113716	2.84%	0.522%
13	11.869	1659	1663	1669	rVB	75021	91451	2.28%	0.420%
14	12.357	1741	1746	1753	rVB5	24457	40228	1.00%	0.185%
15	12.780	1812	1818	1823	rBV	25801	41109	1.03%	0.189%
16	12.910	1835	1840	1843	rBV	4012057	4006595	100.00%	18.407%
17	13.962	2016	2019	2023	rBV	861995	733114	18.30%	3.368%
18	14.121	2037	2046	2050	rBV3	40825	65864	1.64%	0.303%
19	14.727	2145	2149	2154	rBV	42806	52063	1.30%	0.239%
20	15.057	2201	2205	2210	rVB	59584	64947	1.62%	0.298%
21	15.427	2262	2268	2274	rBV	490107	610046	15.23%	2.803%
22	15.856	2336	2341	2347	rVB	65601	96109	2.40%	0.442%
23	15.933	2349	2354	2362	rVV3	47702	79277	1.98%	0.364%
24	16.351	2415	2425	2431	rVB	63237	142470	3.56%	0.655%
25	16.927	2519	2523	2534	rVB3	40905	86082	2.15%	0.395%
26	17.615	2634	2640	2647	rVB3	32441	75394	1.88%	0.346%

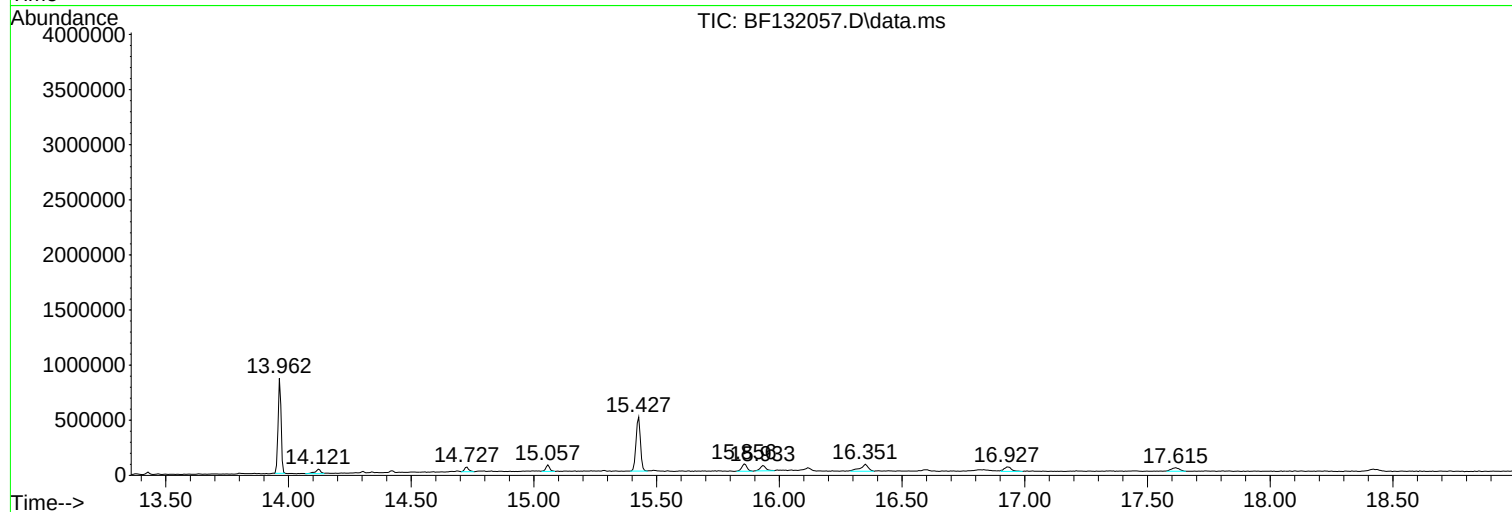
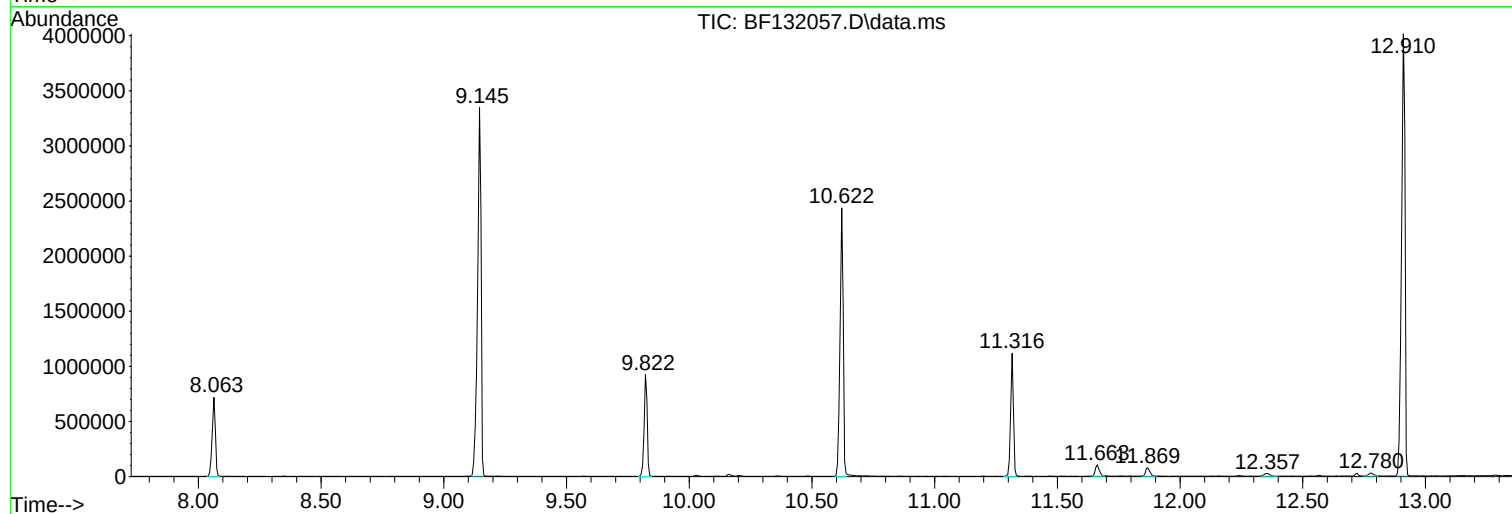
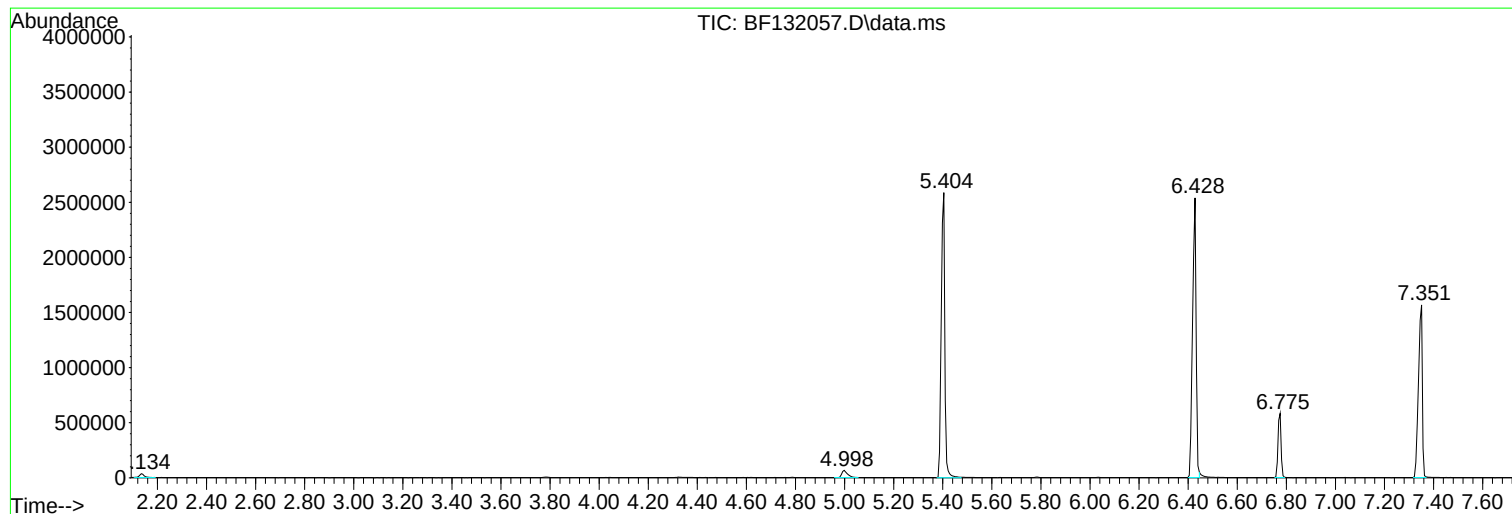
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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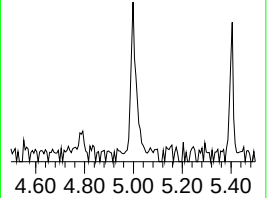
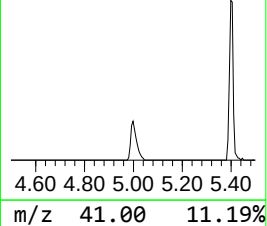
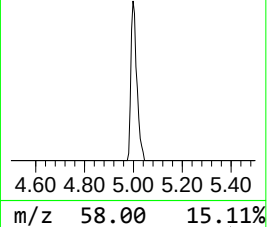
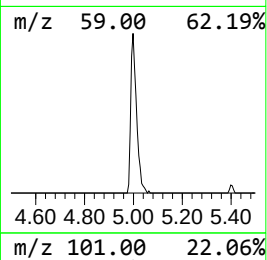
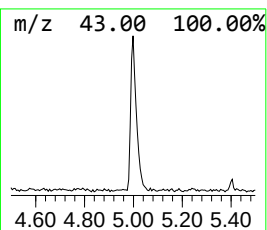
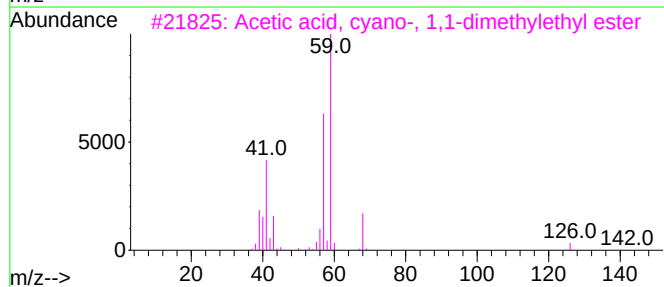
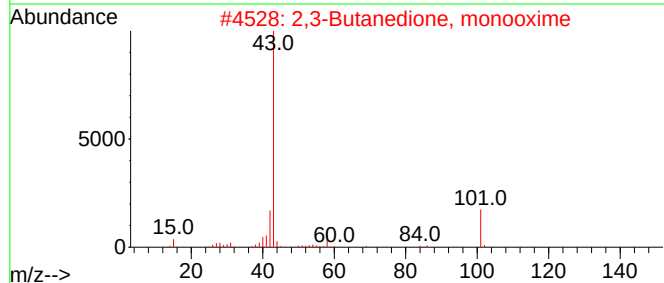
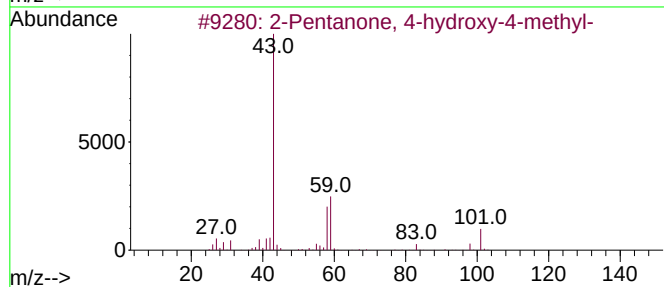
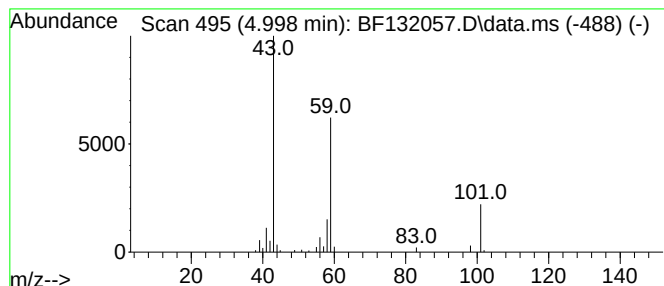
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	4.17 ng	105286	1,4-Dichlorobenzene-d4	6.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9		



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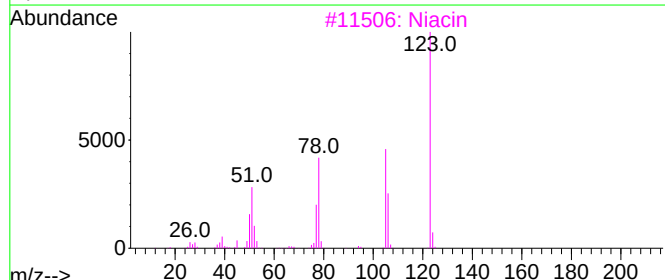
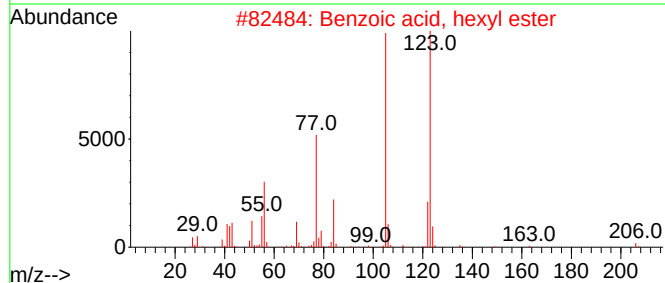
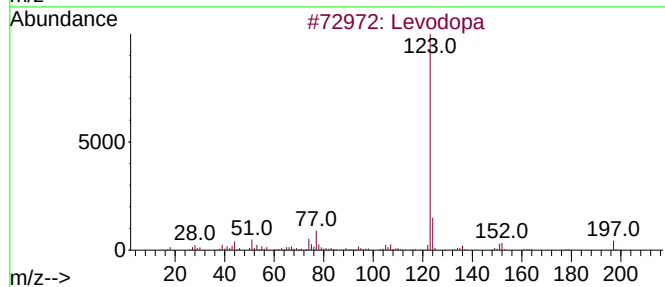
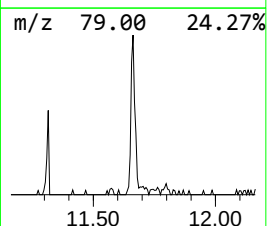
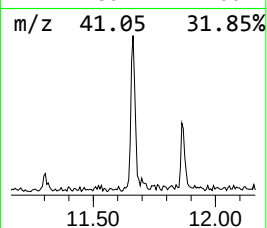
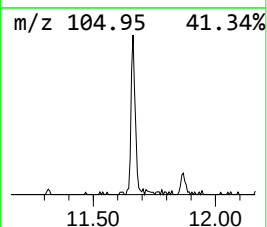
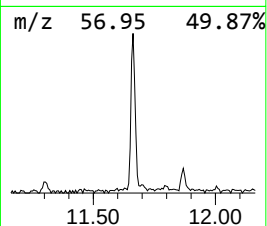
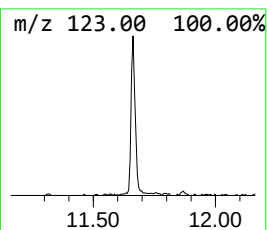
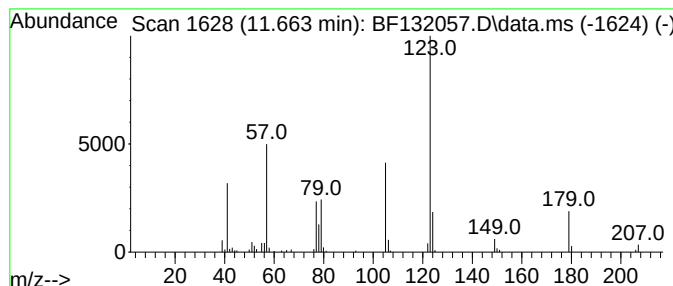
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown11.663 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.663	2.56 ng	113716	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Levodopa	197	C9H11NO4	000059-92-7	28
2			Benzoic acid, hexyl ester	206	C13H18O2	006789-88-4	17
3			Niacin	123	C6H5NO2	000059-67-6	9
4			Propanamide, N-(4-methoxyphenyl)-	179	C10H13NO2	002760-31-8	9
5			4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	9



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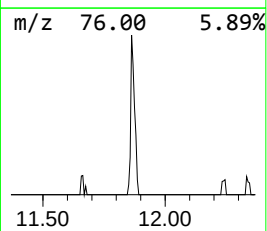
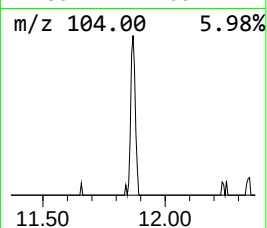
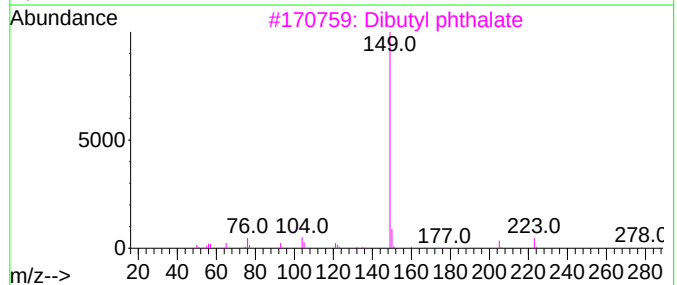
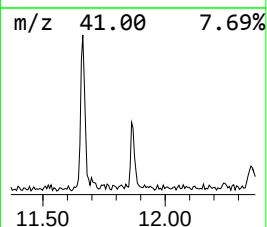
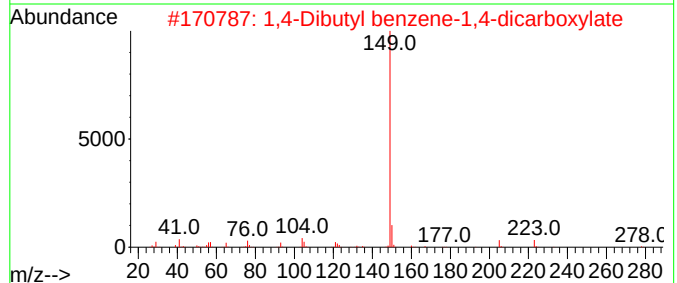
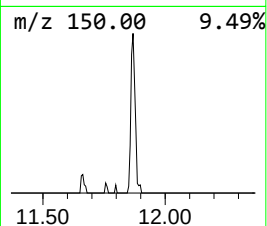
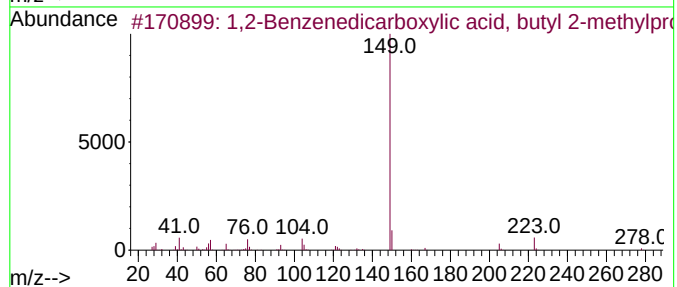
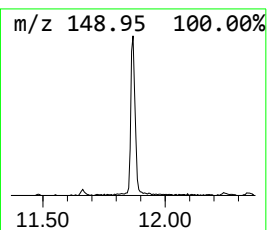
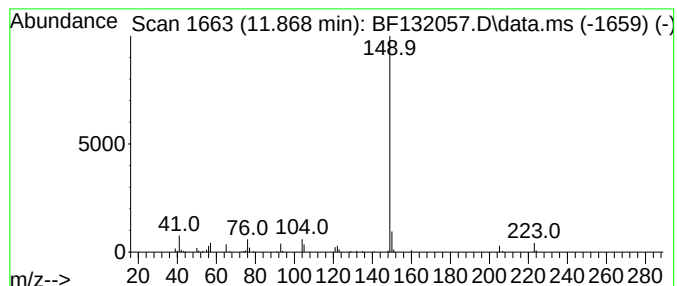
Instrument :
BNA_F
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TIC Integration Parameters: LSCINT.P

Peak Number 3 1,2-Benzenedicarboxylic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.868	2.06 ng	91451	Phenanthrene-d10	11.316	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	90
2	1,4-Dibutyl benzene-1,4-dicarbox...	278	C16H22O4	001962-75-0	90
3	Dibutyl phthalate	278	C16H22O4	000084-74-2	90
4	Phthalic acid, butyl 8-chlorooct...	368	C20H29ClO4	1000356-85-9	83
5	1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	83



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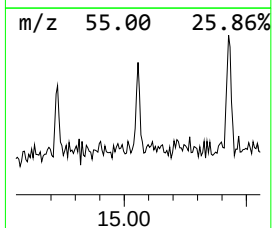
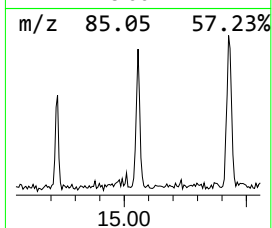
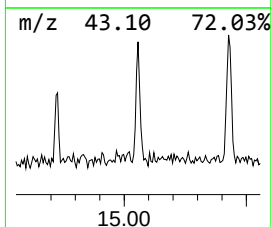
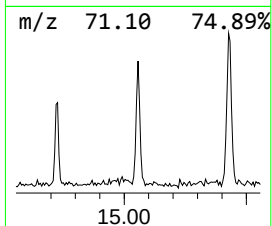
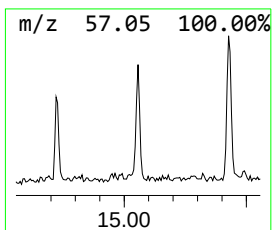
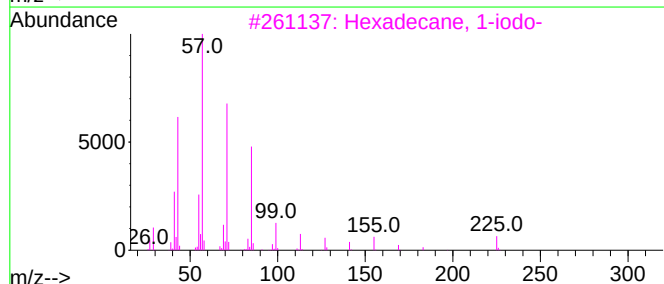
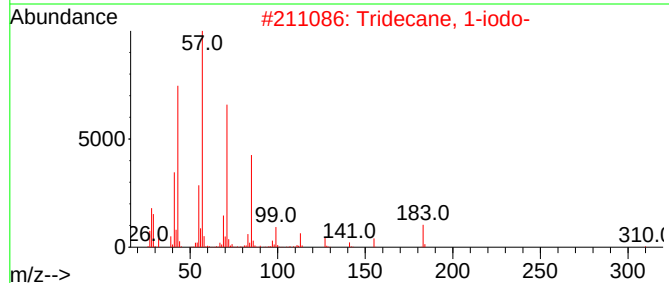
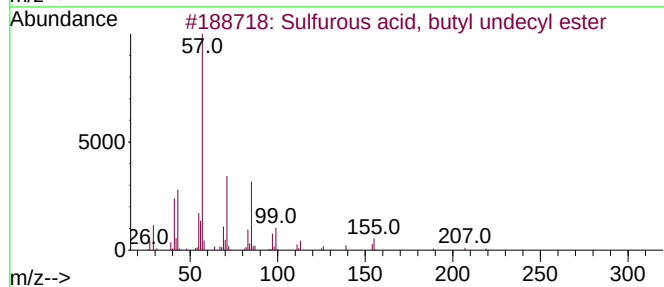
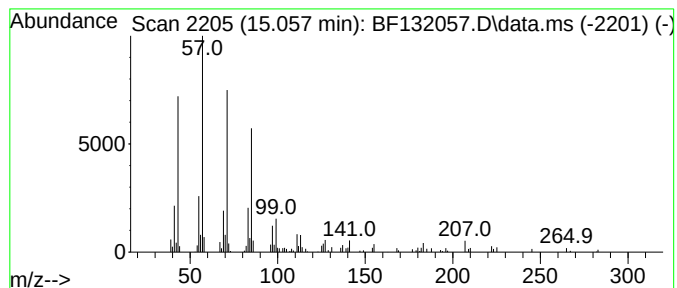
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Peak Number 4 Sulfurous acid, butyl undec... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	2.13 ng	64947	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	80
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
5			Tetratetracontane	619	C44H90	007098-22-8	64



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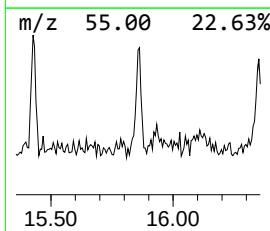
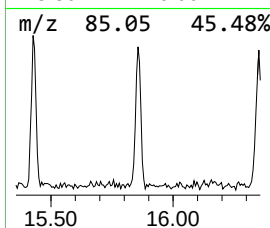
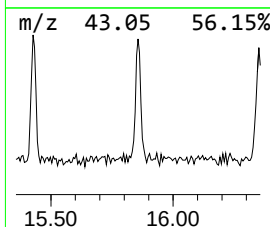
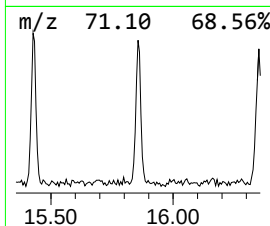
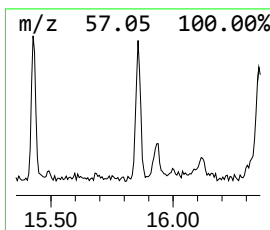
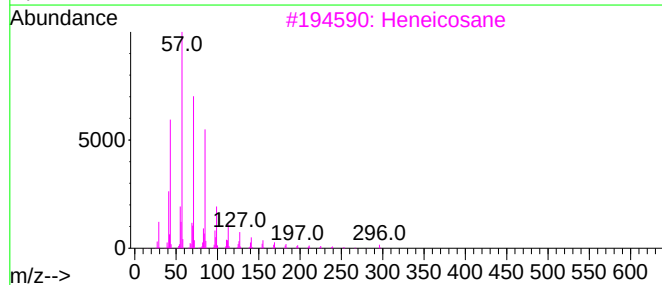
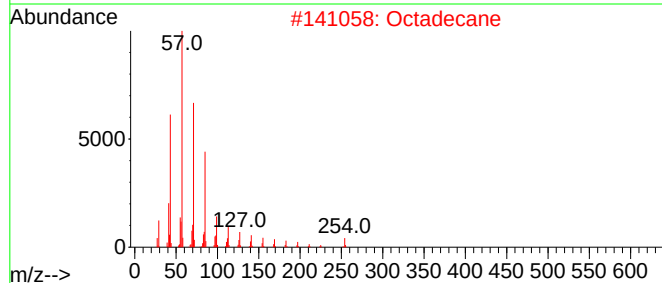
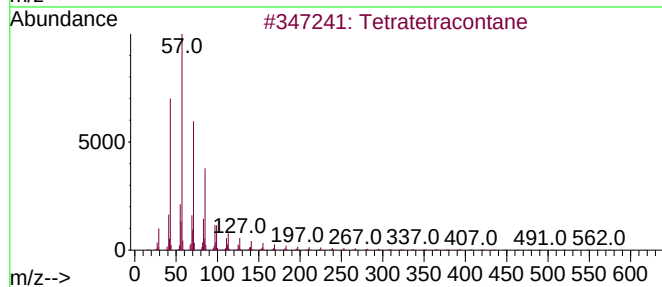
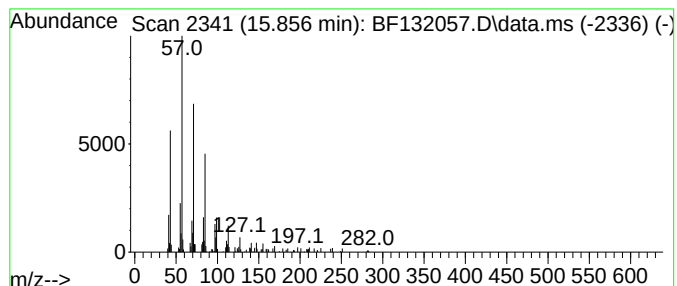
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Peak Number 5 Tetratetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.857	3.15 ng	96109	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Octadecane	254	C18H38	000593-45-3	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5			Octacosane	394	C28H58	000630-02-4	87



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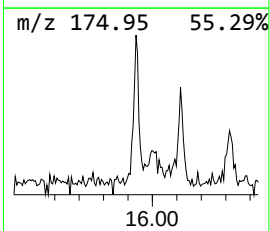
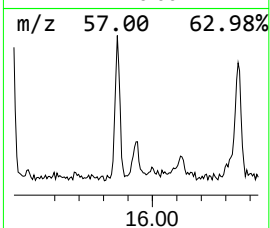
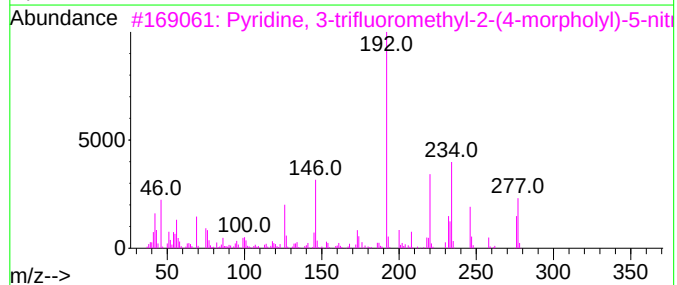
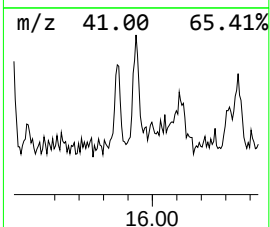
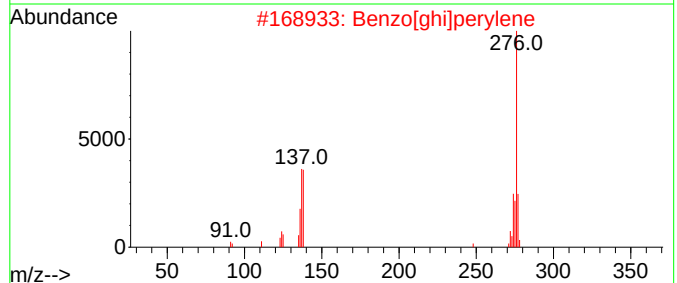
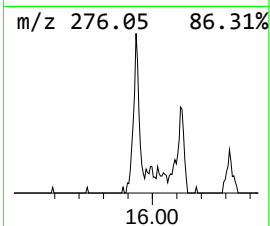
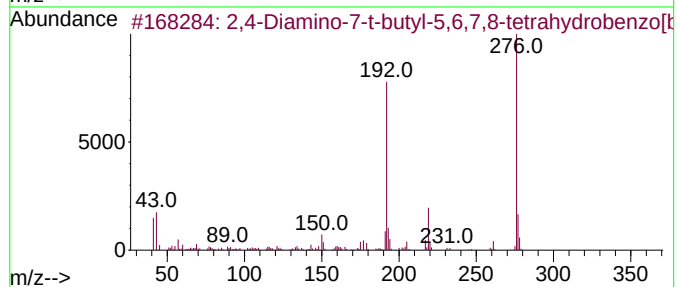
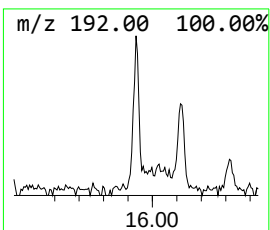
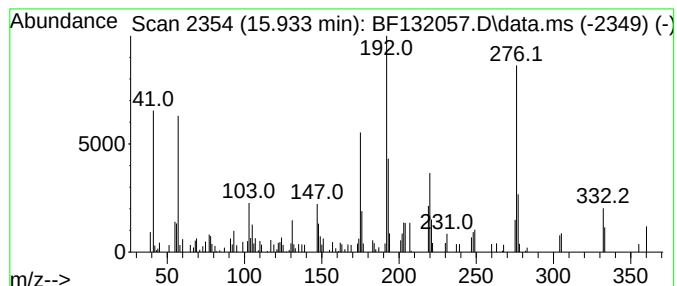
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.933 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.933	2.60 ng	79277	Perylene-d12	15.427

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4-Diamino-7-t-butyl-5,6,7,8-te...	276	C14H20N4S	049620-43-1	43
2		Benzo[ghi]perylene	276	C22H12	000191-24-2	35
3		Pyridine, 3-trifluoromethyl-2-(4...	277	C10H10F3N3O3	288247-15-4	30
4		[1-(4-Fluorophenyl)pyrazol-4-yl]...	192	C10H9FN2O	153863-34-4	25
5		s-1,2,3,4-Tetrahydroisoquinolin...	299	C18H21NO3	1000128-00-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011323\
Data File : BF132057.D
Acq On : 13 Jan 2023 13:50
Operator : CG\JU
Sample : PB150221BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

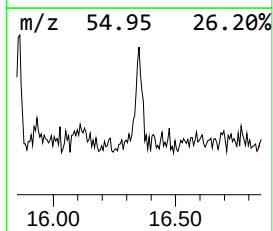
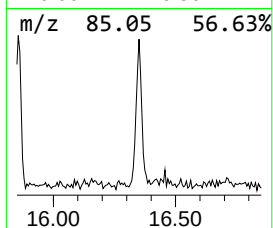
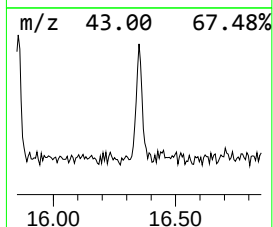
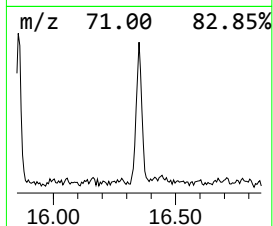
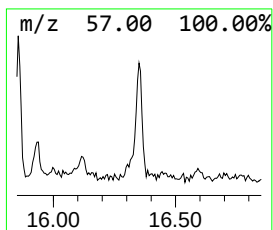
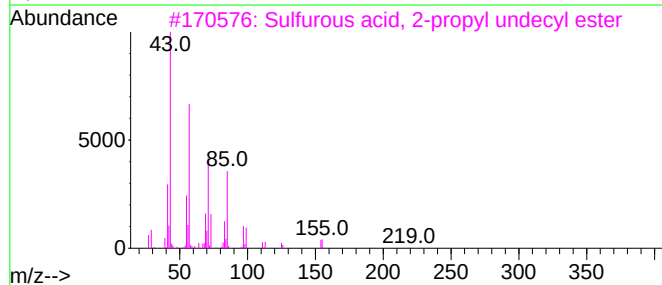
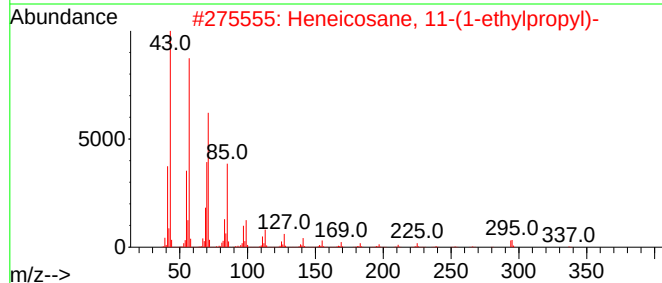
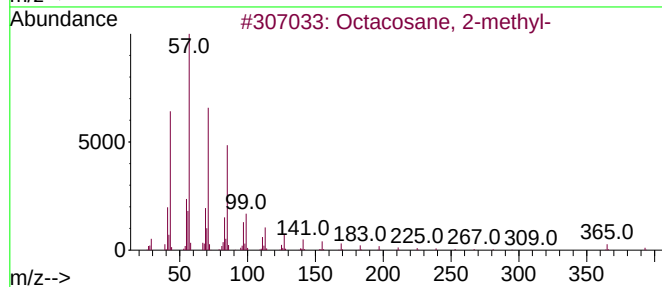
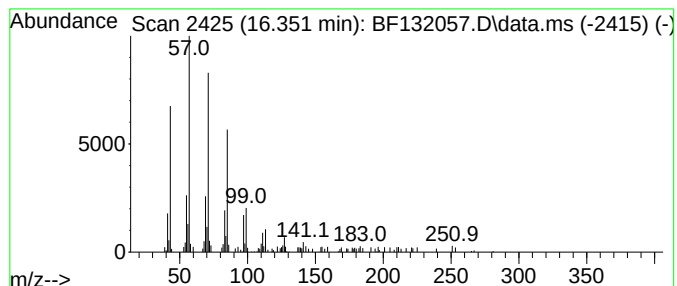
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.351	4.67 ng	142470	Perylene-d12	15.427	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
3	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	86
4	Octacosane	394	C28H58	000630-02-4	83
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011323\
Data File : BF132057.D
Acq On : 13 Jan 2023 13:50
Operator : CG\JU
Sample : PB150221BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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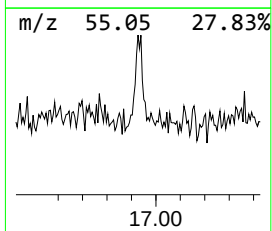
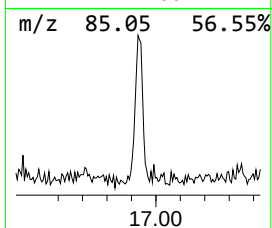
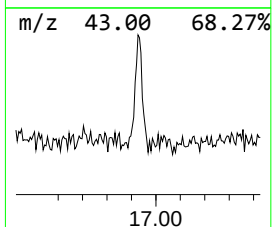
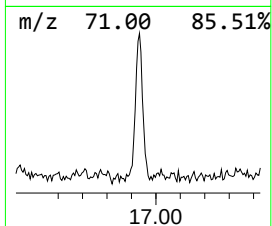
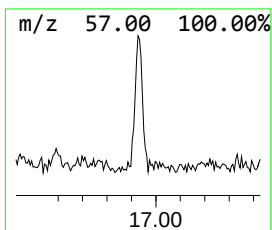
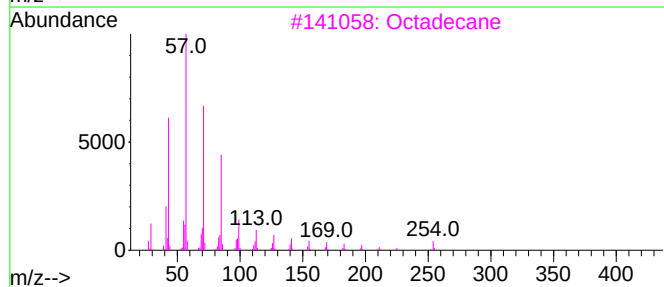
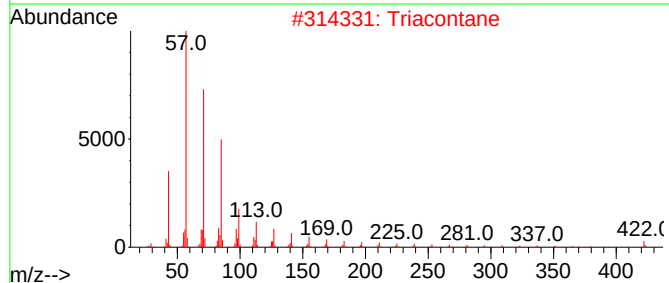
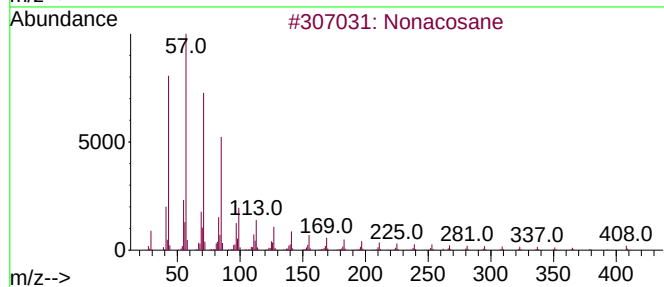
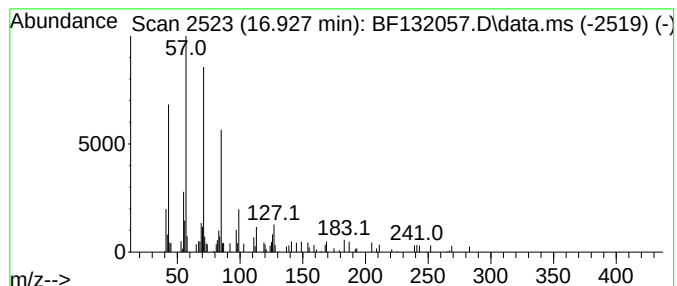
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.927	2.82 ng	86082	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacosane	408	C29H60	000630-03-5	90
2			Triacontane	422	C30H62	000638-68-6	90
3			Octadecane	254	C18H38	000593-45-3	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Pentacosane	352	C25H52	000629-99-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011323\
Data File : BF132057.D
Acq On : 13 Jan 2023 13:50
Operator : CG\JU
Sample : PB150221BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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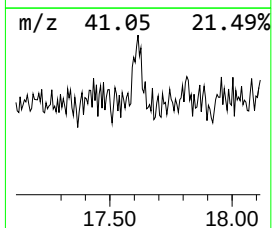
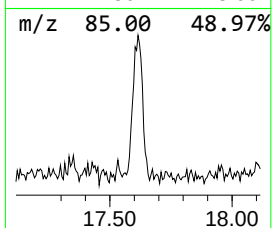
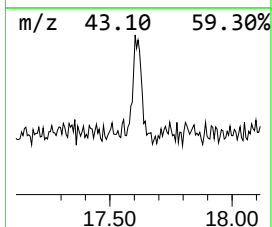
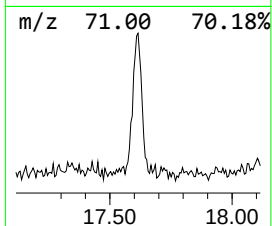
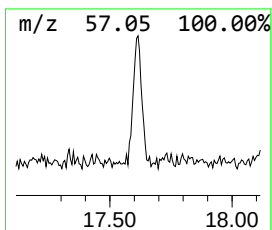
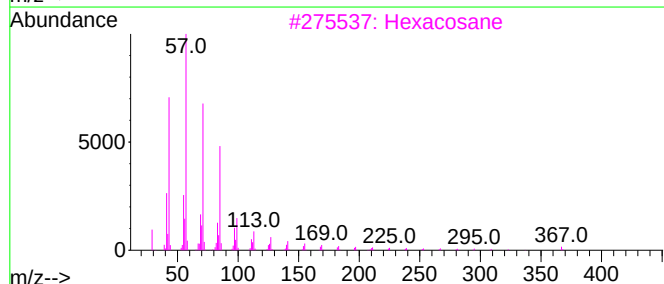
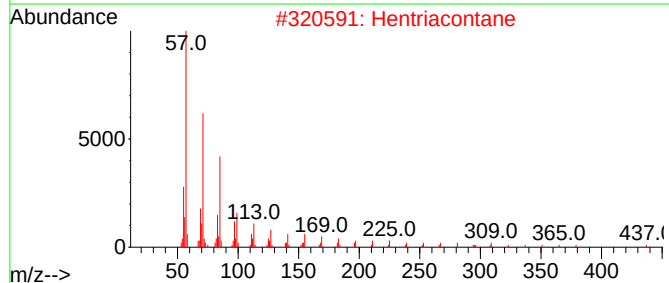
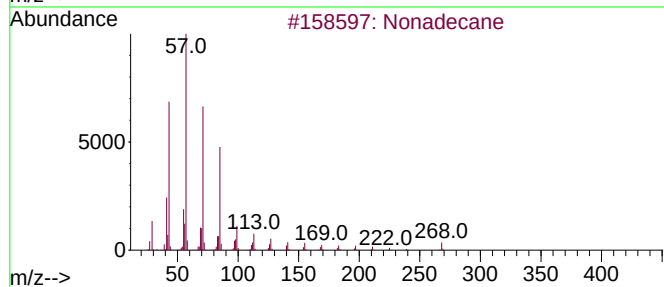
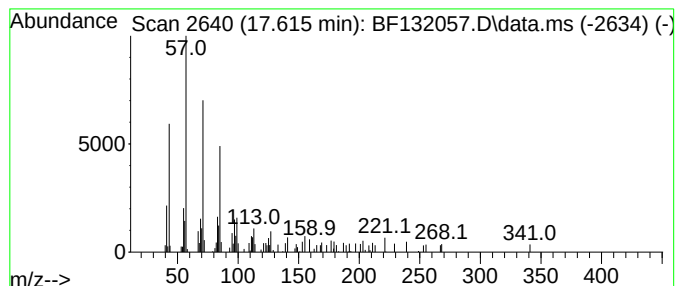
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.615	2.47 ng	75394	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	97
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011323\
Data File : BF132057.D
Acq On : 13 Jan 2023 13:50
Operator : CG\JU
Sample : PB150221BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150221BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.998	4.2	ng	105286	1	6.775	504528	20.0
unknown11.663	11.663	2.6	ng	113716	4	11.316	889194	20.0
1,2-Benzenedica...	11.868	2.1	ng	91451	4	11.316	889194	20.0
Sulfurous acid,...	15.057	2.1	ng	64947	6	15.427	610046	20.0
Tetratetracontane	15.857	3.1	ng	96109	6	15.427	610046	20.0
unknown15.933	15.933	2.6	ng	79277	6	15.427	610046	20.0
Octacosane, 2-m...	16.351	4.7	ng	142470	6	15.427	610046	20.0
Nonacosane	16.927	2.8	ng	86082	6	15.427	610046	20.0
Nonadecane	17.615	2.5	ng	75394	6	15.427	610046	20.0