

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032224\
 Data File : BF137678.D
 Acq On : 22 Mar 2024 13:09
 Operator : CG\JU
 Sample : PB159737BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159737BL

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: BF137678.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	18	rVB	68012	89829	1.32%	0.207%
2	4.957	484	488	502	rBV	159653	275802	4.05%	0.637%
3	5.351	550	555	558	rBV	5105692	5774399	84.81%	13.328%
4	6.369	723	728	731	rBV	4639630	5928239	87.07%	13.683%
5	6.728	785	789	806	rBV	1356438	1353805	19.88%	3.125%
6	7.292	880	885	888	rBV	3534446	3815817	56.05%	8.807%
7	8.004	1002	1006	1025	rBV	1738584	1808355	26.56%	4.174%
8	9.086	1184	1190	1193	rBV	6530403	6808272	100.00%	15.714%
9	9.757	1299	1304	1321	rBV	2260338	2053225	30.16%	4.739%
10	10.551	1434	1439	1459	rBV	3880371	3829976	56.25%	8.840%
11	11.239	1553	1556	1567	rBV	1903179	1919369	28.19%	4.430%
12	12.651	1793	1796	1802	rVB	230747	180634	2.65%	0.417%
13	12.833	1822	1827	1830	rBV	6011251	5893904	86.57%	13.604%
14	13.357	1912	1916	1921	rBV	155667	124300	1.83%	0.287%
15	13.874	2001	2004	2017	rBV	1131891	1179984	17.33%	2.724%
16	14.651	2132	2136	2139	rBV	98713	102841	1.51%	0.237%
17	14.968	2187	2190	2197	rVB	126753	139003	2.04%	0.321%
18	15.298	2241	2246	2250	rBV	773489	1075933	15.80%	2.483%
19	15.739	2316	2321	2327	rBV	143736	215903	3.17%	0.498%
20	16.215	2397	2402	2408	rBV	128325	220609	3.24%	0.509%
21	16.374	2421	2429	2430	rBV4	47192	89727	1.32%	0.207%
22	16.774	2491	2497	2505	rVB	90074	184430	2.71%	0.426%
23	17.433	2602	2609	2619	rVB3	70105	165480	2.43%	0.382%
24	18.215	2735	2742	2749	rVB6	34562	95601	1.40%	0.221%

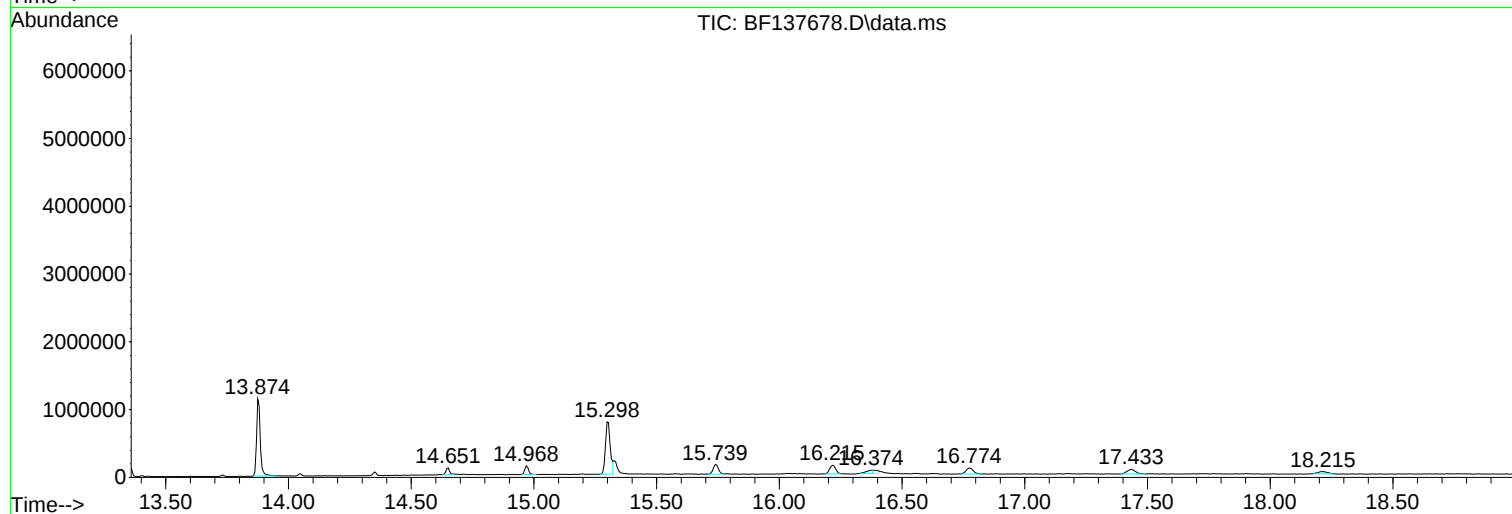
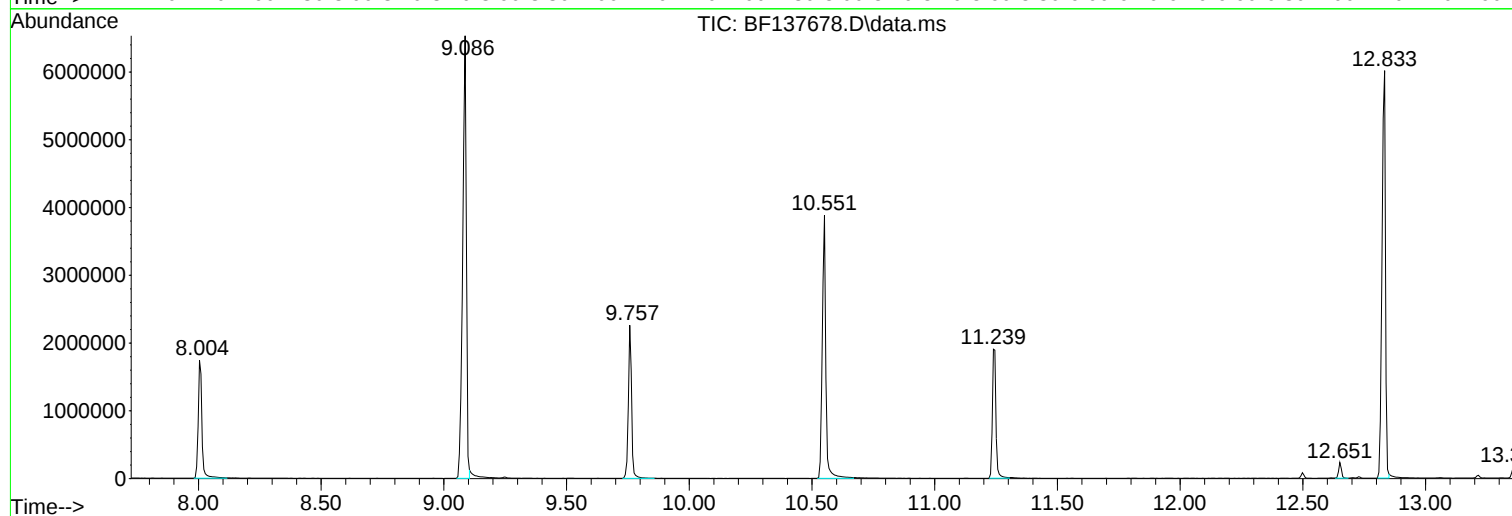
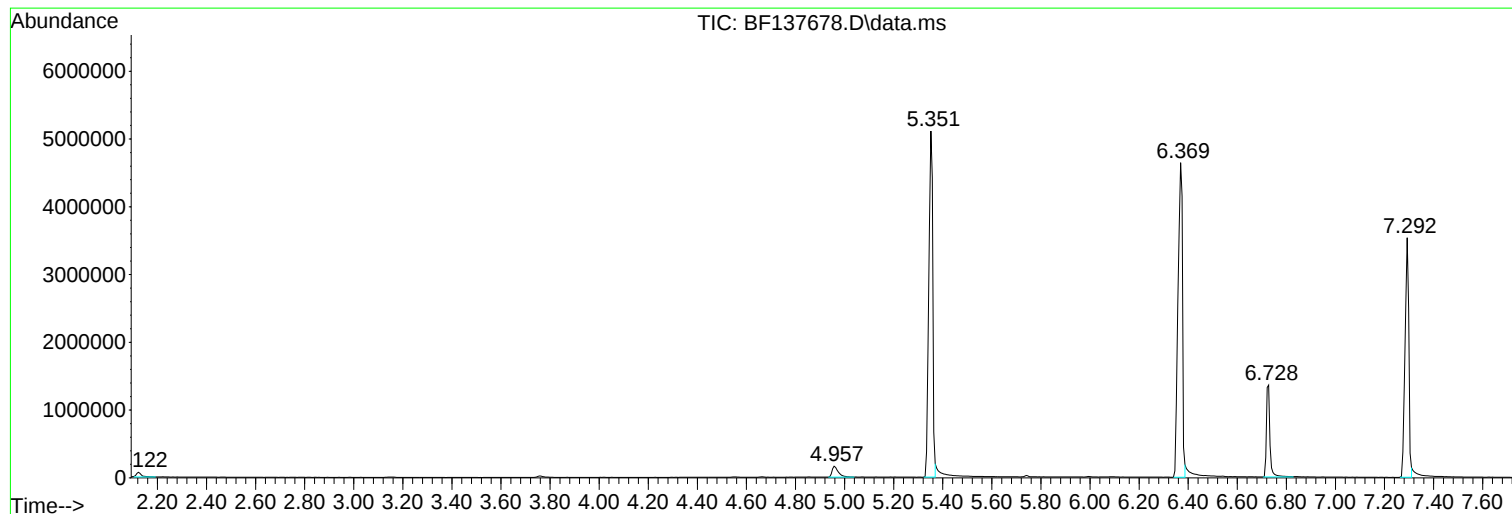
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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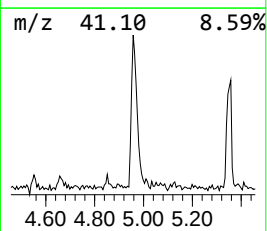
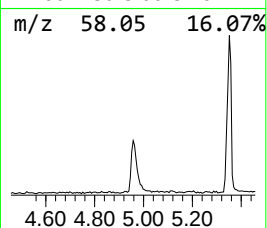
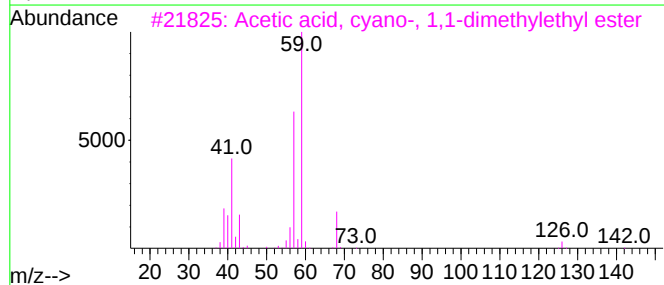
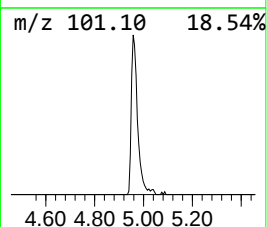
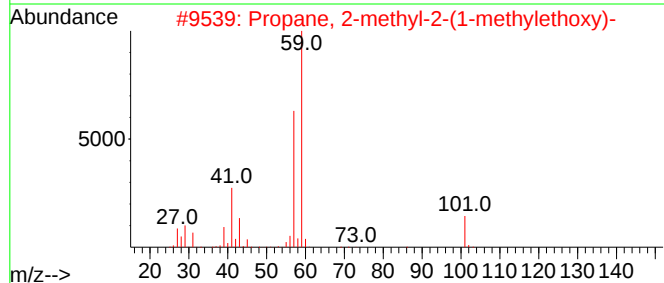
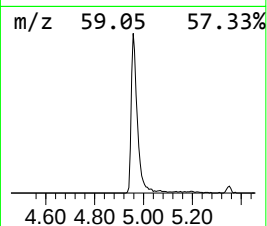
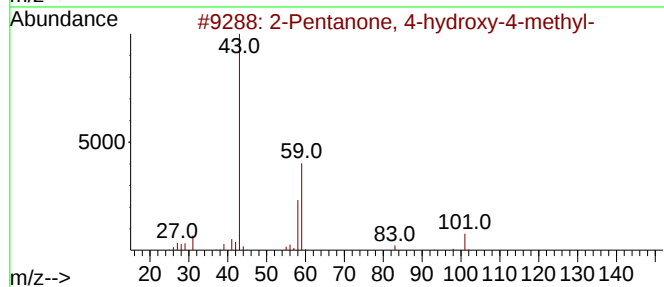
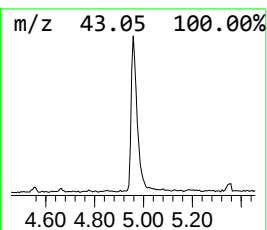
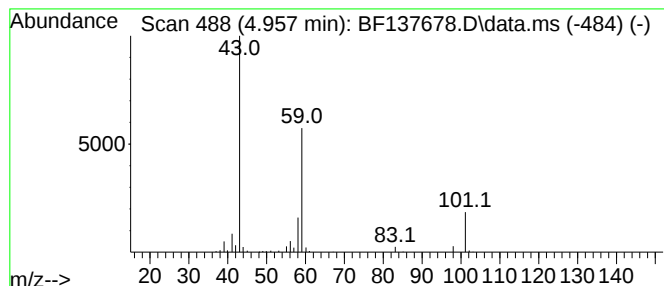
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.957	4.07 ng	275802	1,4-Dichlorobenzene-d4	6.728	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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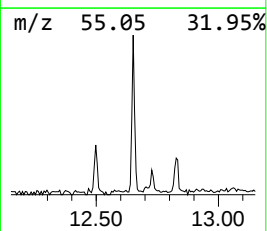
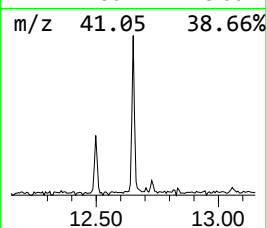
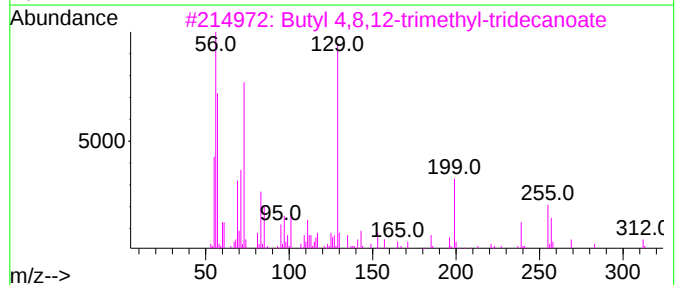
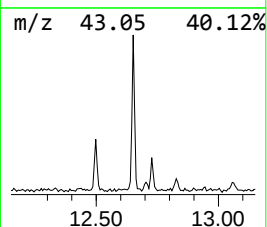
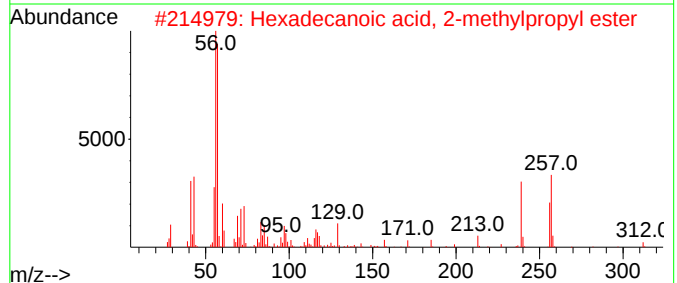
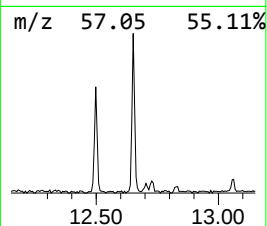
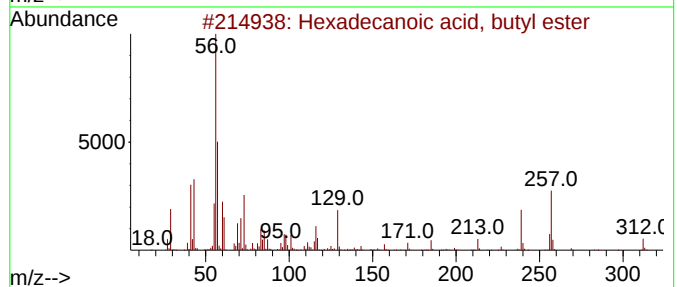
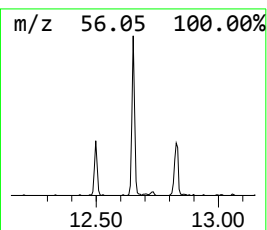
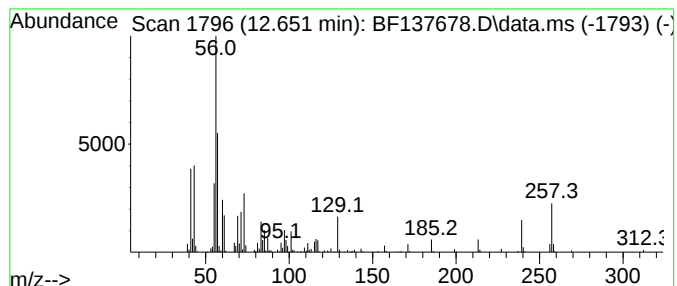
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	3.06 ng	180634	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	78
3			Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	40
4			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	38
5			Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35



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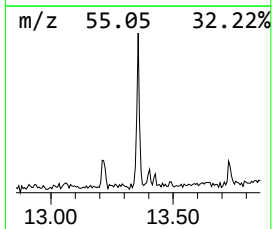
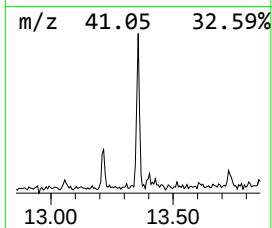
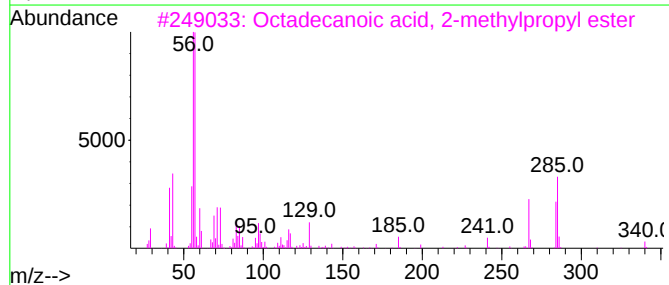
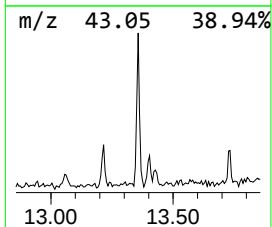
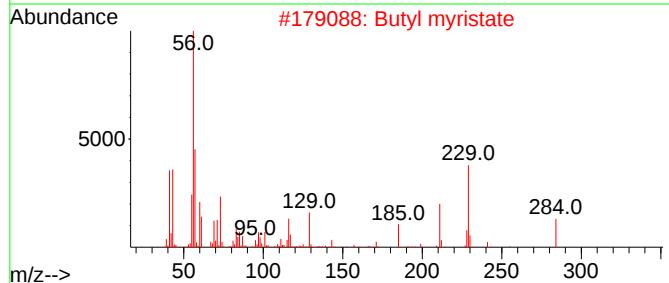
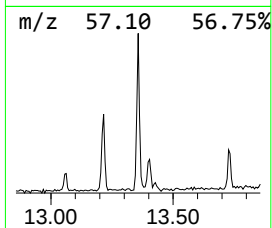
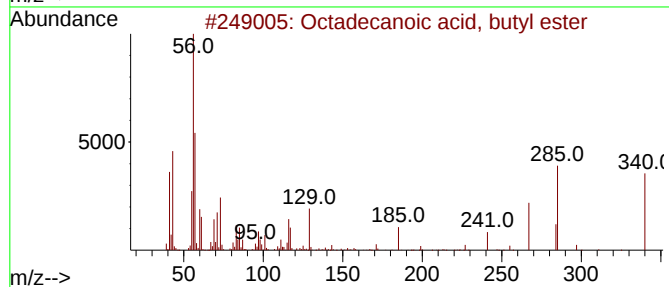
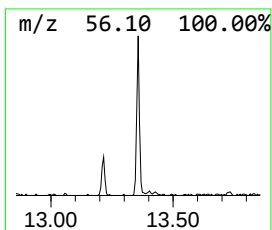
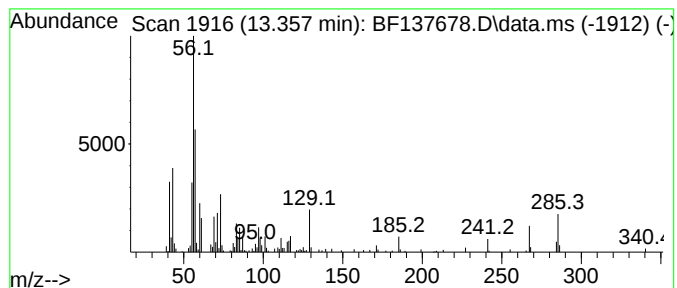
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.357	2.11 ng	124300	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	95
2			Butyl myristate	284	C18H36O2	000110-36-1	80
3			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	64
4			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35
5			Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



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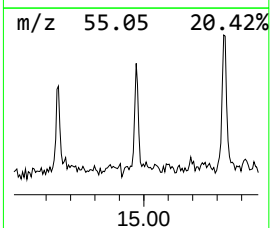
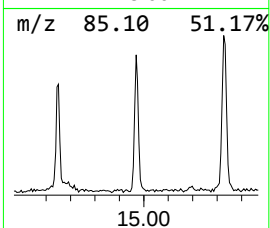
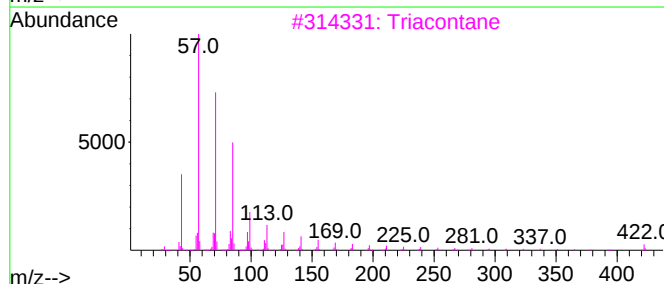
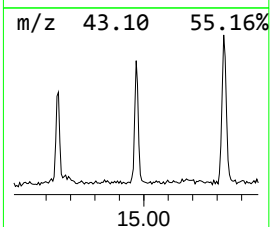
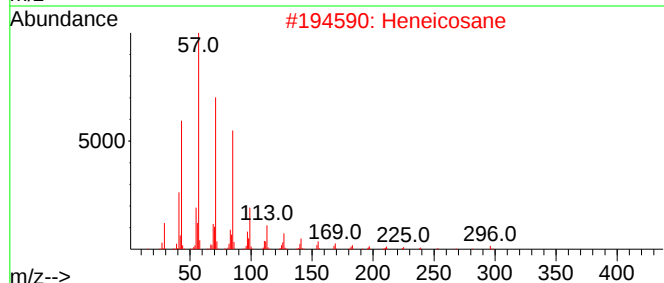
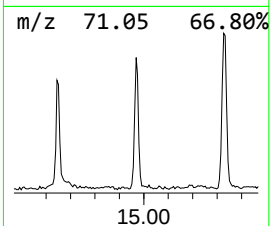
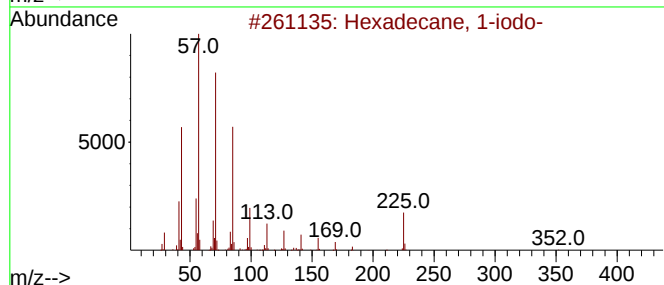
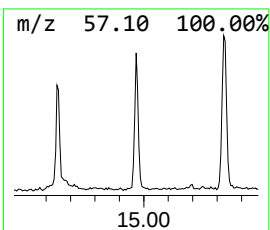
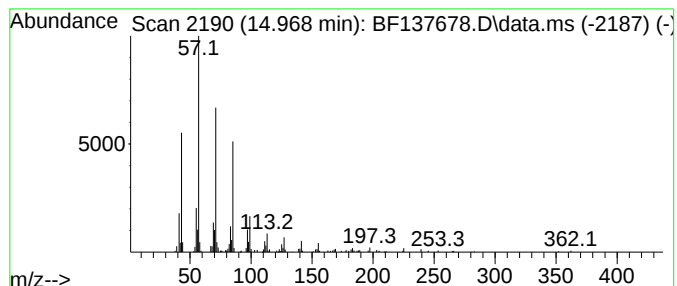
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Peak Number 4 Hexadecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.969	2.58 ng	139003	Perylene-d12	15.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
2		Heneicosane	296	C21H44	000629-94-7	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Tetracosane	338	C24H50	000646-31-1	91



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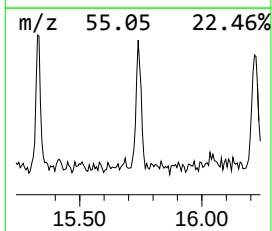
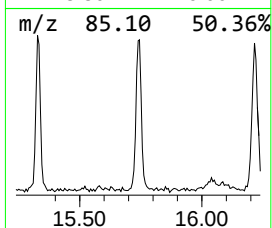
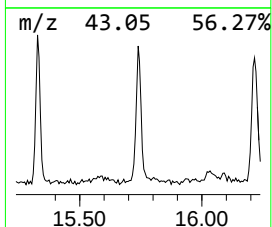
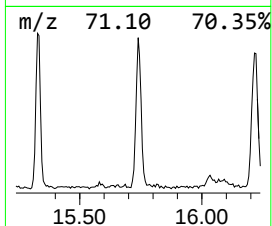
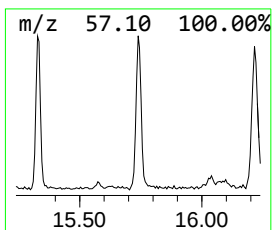
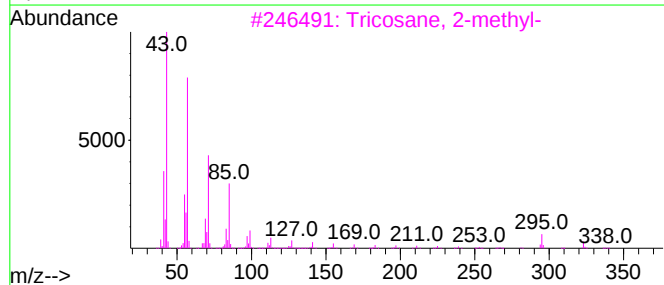
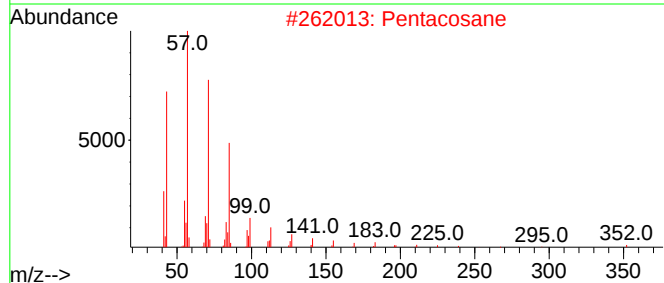
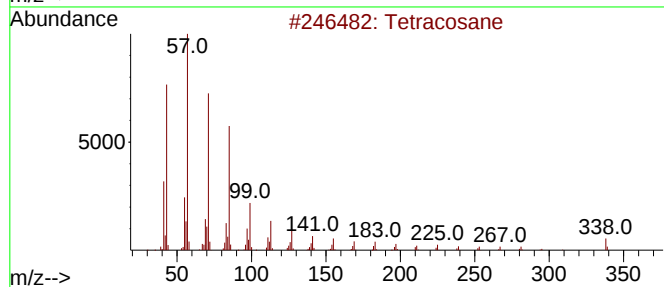
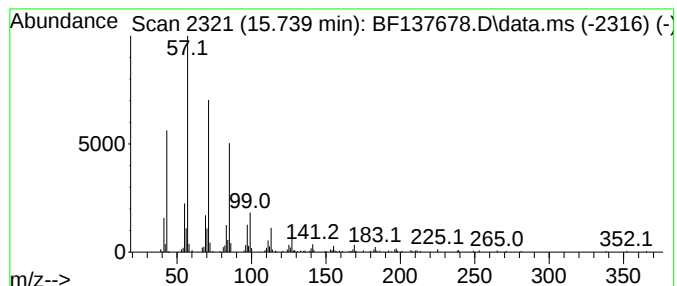
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	4.01 ng	215903	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	97
2			Pentacosane	352	C25H52	000629-99-2	94
3			Tricosane, 2-methyl-	338	C24H50	001928-30-9	93
4			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87



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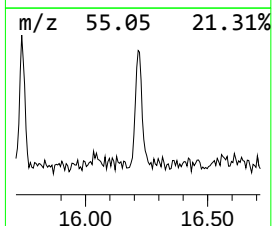
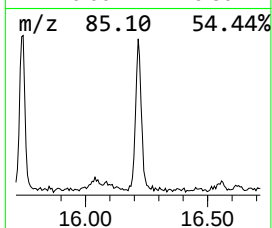
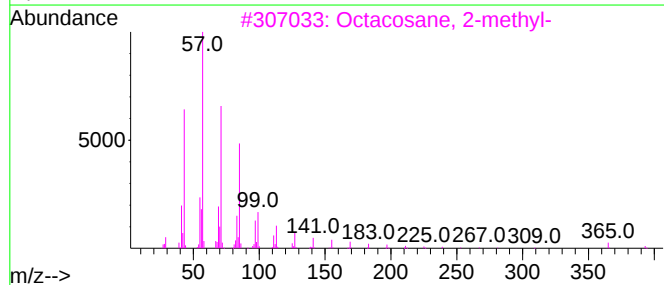
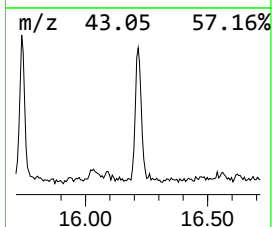
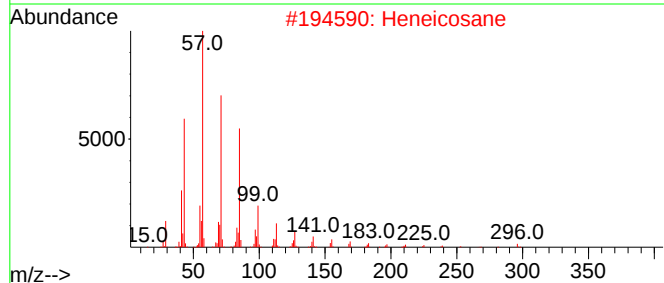
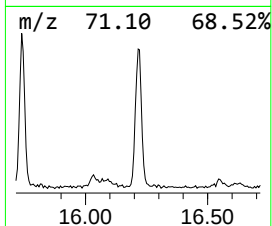
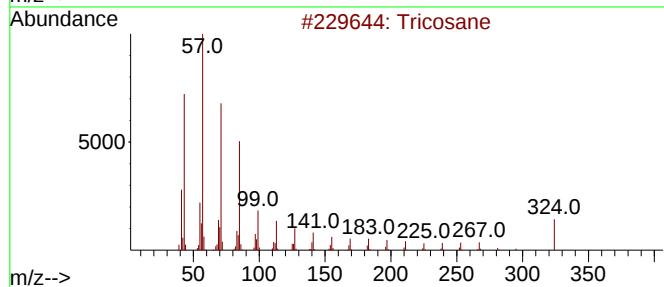
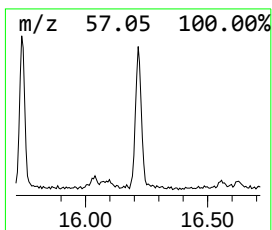
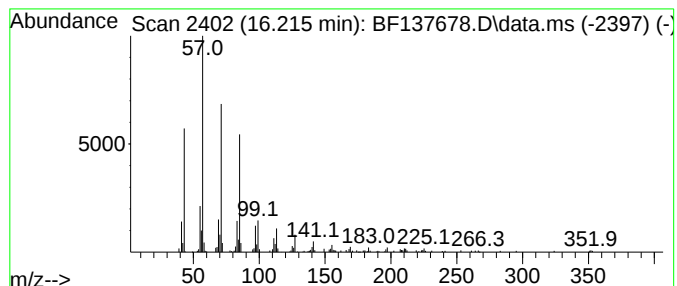
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tricosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	4.10 ng	220609	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	93
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Tetracosane	338	C24H50	000646-31-1	90
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032224\
Data File : BF137678.D
Acq On : 22 Mar 2024 13:09
Operator : CG\JU
Sample : PB159737BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159737BL

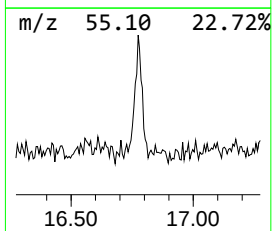
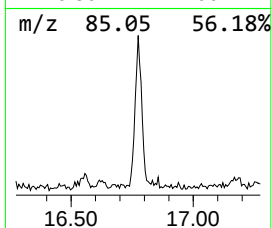
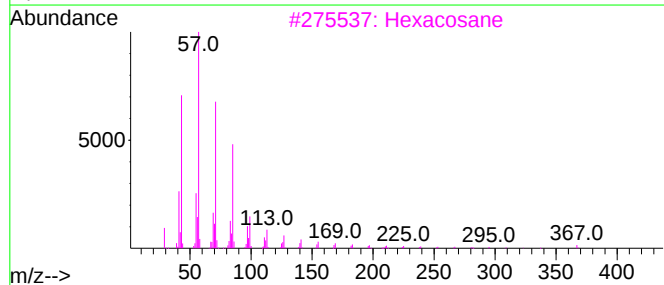
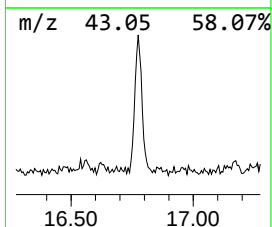
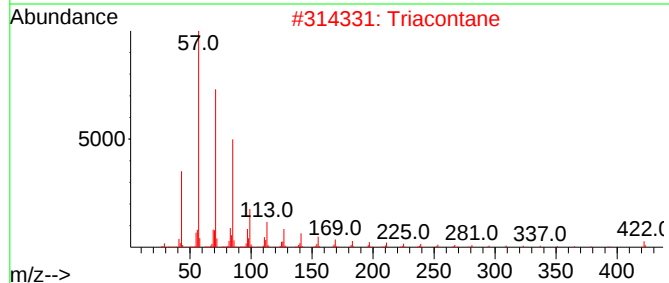
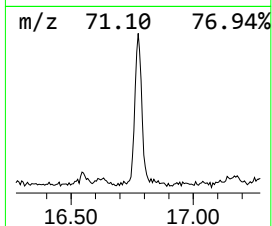
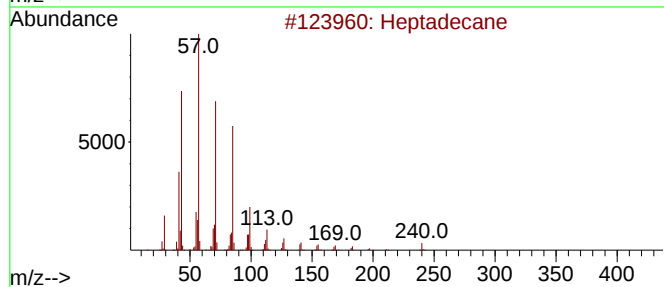
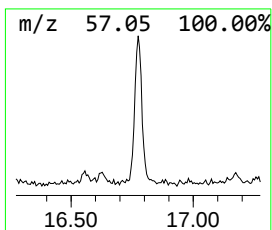
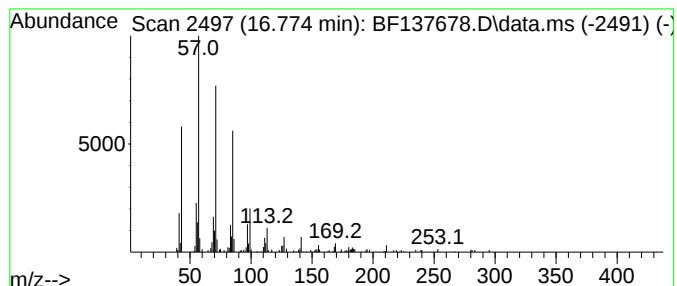
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	3.43 ng	184430	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	94
2			Triacontane	422	C30H62	000638-68-6	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032224\
Data File : BF137678.D
Acq On : 22 Mar 2024 13:09
Operator : CG\JU
Sample : PB159737BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159737BL

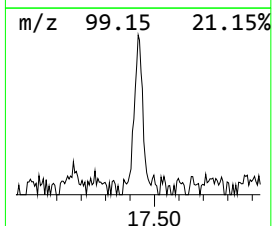
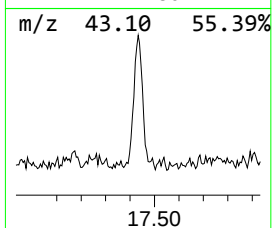
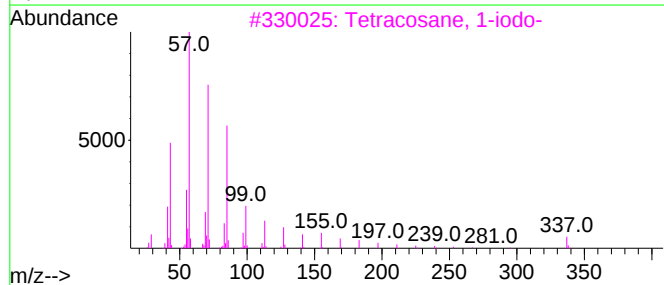
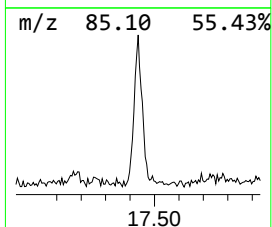
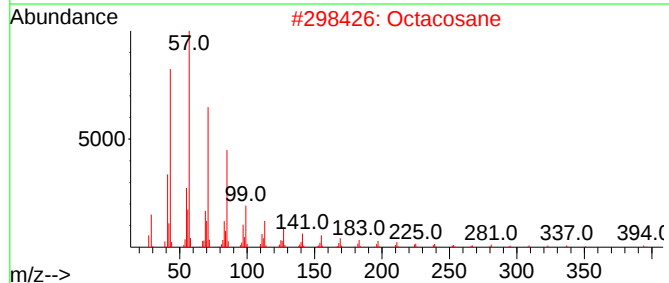
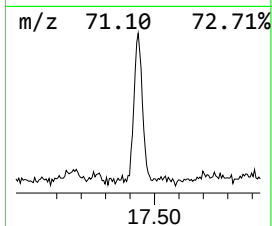
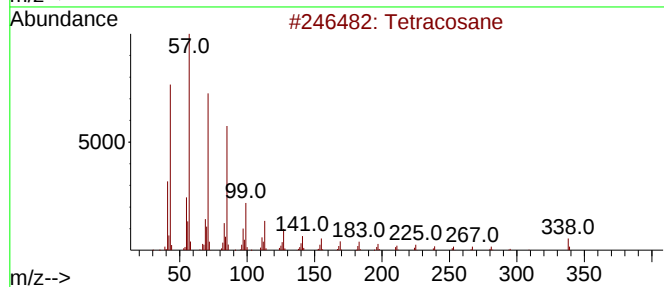
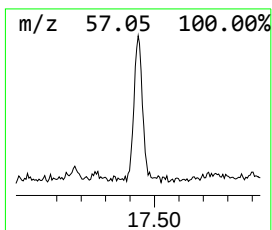
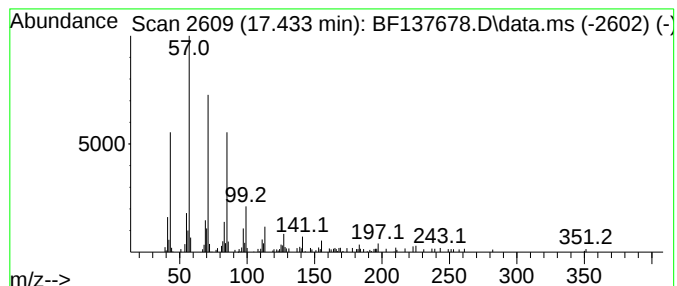
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.433	3.08 ng	165480	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	90
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032224\
Data File : BF137678.D
Acq On : 22 Mar 2024 13:09
Operator : CG\JU
Sample : PB159737BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159737BL

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	4.1	ng	275802	1	6.728	1353810	20.0
Hexadecanoic ac...	12.651	3.1	ng	180634	5	13.874	1179980	20.0
Octadecanoic ac...	13.357	2.1	ng	124300	5	13.874	1179980	20.0
Hexadecane, 1-i...	14.969	2.6	ng	139003	6	15.304	1075930	20.0
Tetracosane	15.739	4.0	ng	215903	6	15.304	1075930	20.0
Tricosane	16.215	4.1	ng	220609	6	15.304	1075930	20.0
Heptadecane	16.774	3.4	ng	184430	6	15.304	1075930	20.0
Tetracosane, 1-...	17.433	3.1	ng	165480	6	15.304	1075930	20.0