

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011024\
 Data File : BG060296.D
 Acq On : 10 Jan 2024 11:34
 Operator : MA/JU
 Sample : P1067-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SP-A-COMP(0-8)

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_G\Methods\8270-BG010824.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060296.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.036	325	331	338	rBV	155370	237729	1.91%	0.360%
2	5.506	404	411	426	rBV	2780057	4340565	34.78%	6.567%
3	7.098	673	682	693	rBV	2873410	5031868	40.32%	7.613%
4	7.933	815	824	833	rBV	741693	1240946	9.94%	1.878%
5	9.090	1012	1021	1036	rBV	1859180	3271509	26.22%	4.950%
6	10.735	1291	1301	1308	rBV	996657	1775199	14.23%	2.686%
7	13.191	1711	1719	1727	rBV	5758444	8862453	71.02%	13.409%
8	14.566	1946	1953	1960	rBV	1784914	2767298	22.18%	4.187%
9	16.059	2200	2207	2214	rBV	4291764	6618211	53.04%	10.013%
10	17.316	2415	2421	2430	rVB	2257573	3350159	26.85%	5.069%
11	18.203	2568	2572	2589	rVB4	494224	1207011	9.67%	1.826%
12	19.314	2753	2761	2771	rBV4	277213	832635	6.67%	1.260%
13	19.478	2785	2789	2809	rVB2	605523	1453145	11.64%	2.199%
14	19.936	2861	2867	2876	rBV	9127013	12478731	100.00%	18.880%
15	20.571	2968	2975	2988	rVB	581238	1401001	11.23%	2.120%
16	20.729	2999	3002	3006	rVB2	134176	143055	1.15%	0.216%
17	21.229	3082	3087	3095	rBV2	458810	784611	6.29%	1.187%
18	21.581	3140	3147	3152	rBV	2208917	3977206	31.87%	6.017%
19	21.769	3175	3179	3182	rVB2	111276	136007	1.09%	0.206%
20	22.363	3277	3280	3290	rVB3	124907	238583	1.91%	0.361%
21	22.862	3357	3365	3375	rVB2	430196	1243928	9.97%	1.882%
22	24.278	3598	3606	3620	rVB5	299506	1051782	8.43%	1.591%
23	24.748	3677	3686	3701	rBV	1155673	3651023	29.26%	5.524%

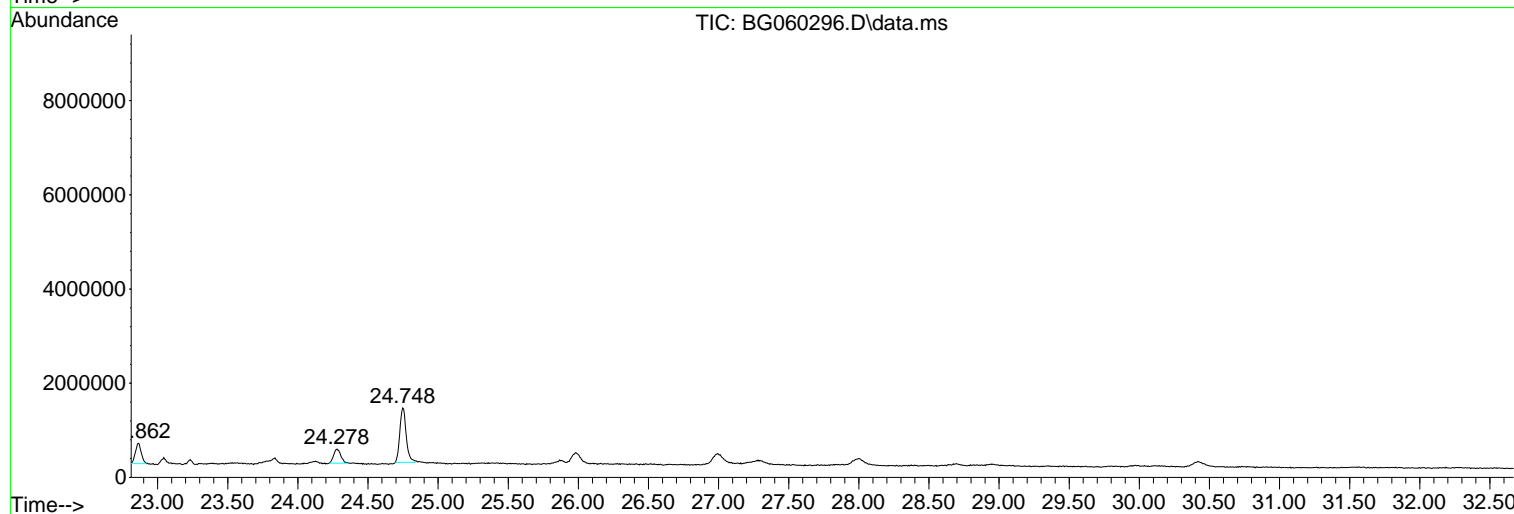
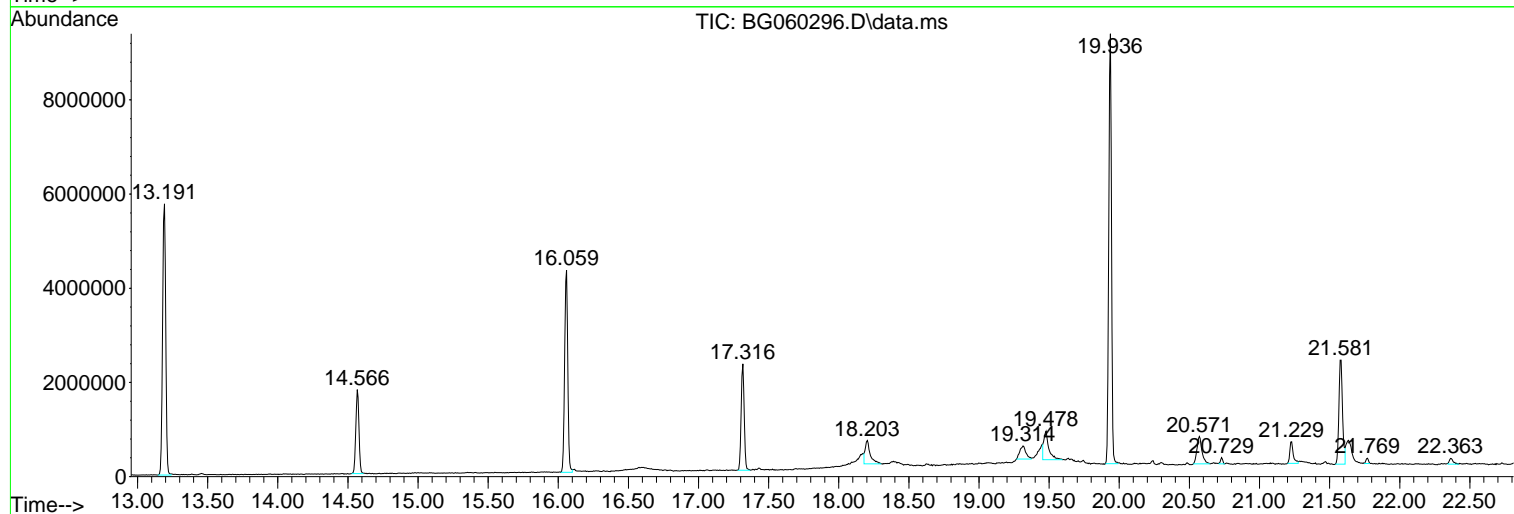
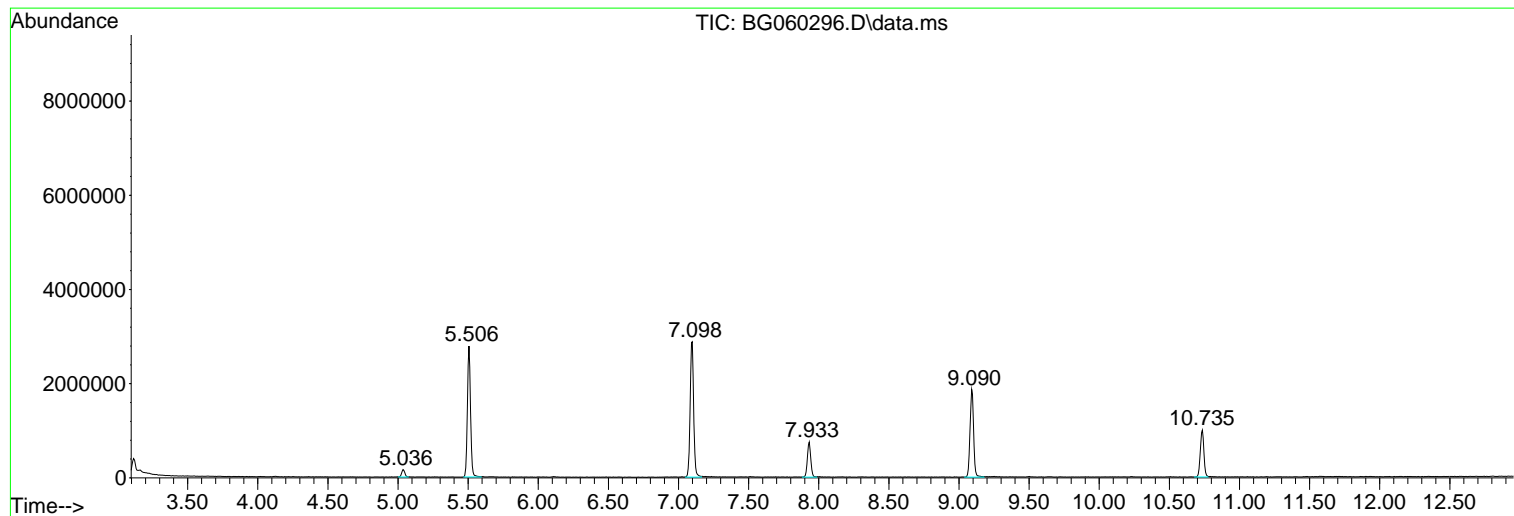
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Instrument :
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ClientSampleId :
SP-A-COMP(0-8)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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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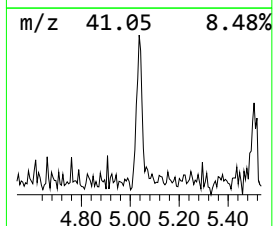
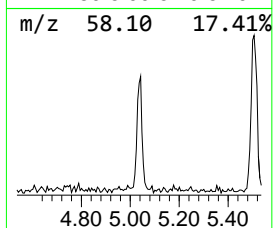
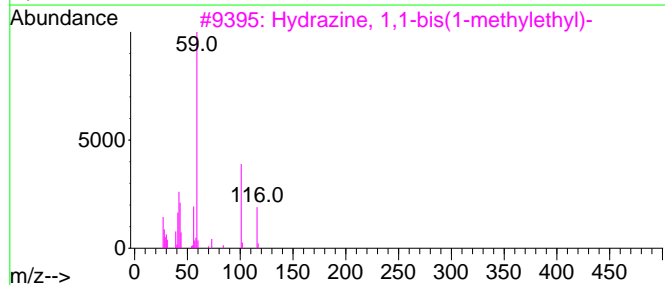
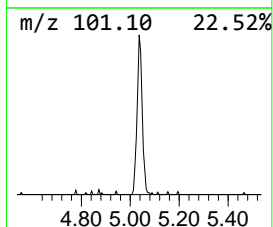
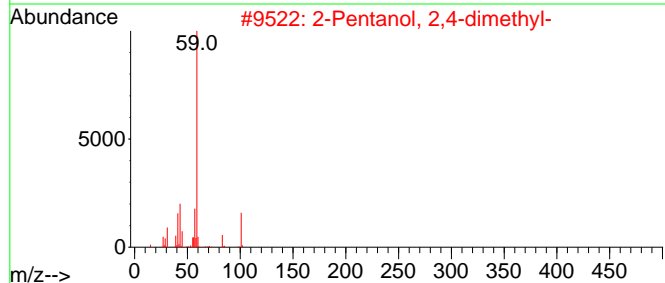
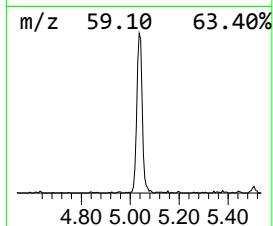
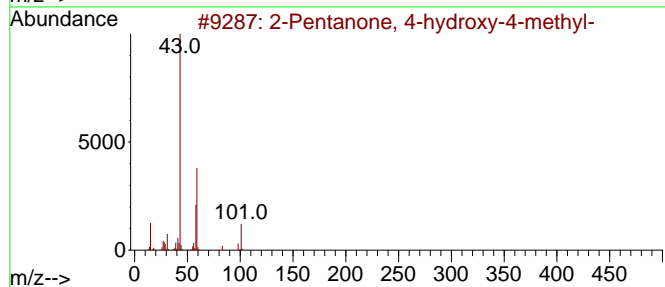
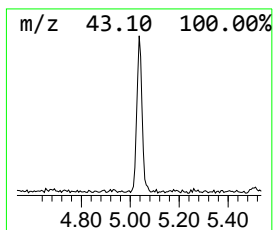
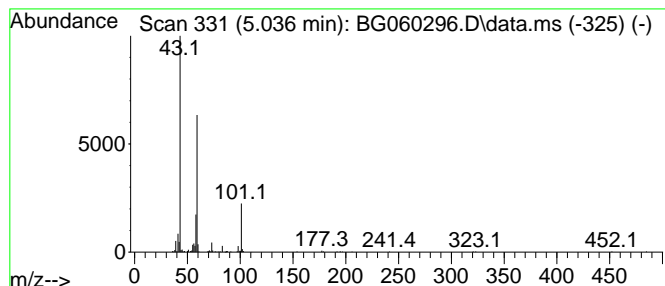
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.036	3.83 ng	237729	1,4-Dichlorobenzene-d4	7.933

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	37
3		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33
4		Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	25
5		5-Deoxy-.alpha.-d-xylofuranose, ...	174	C8H14O4	1000314-09-4	25



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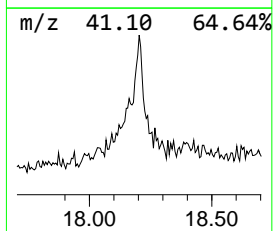
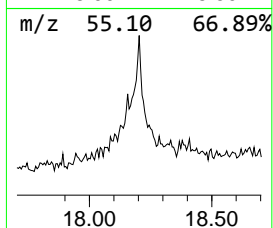
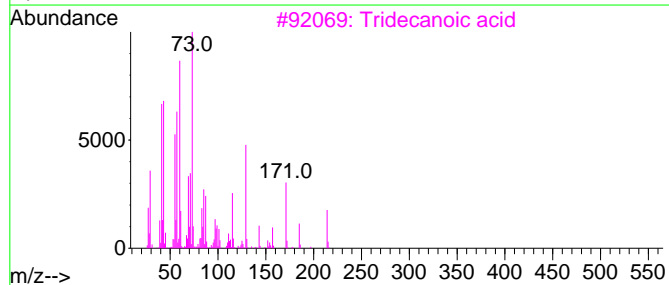
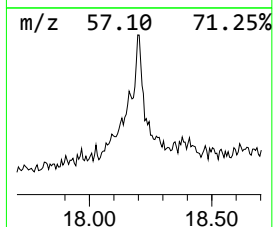
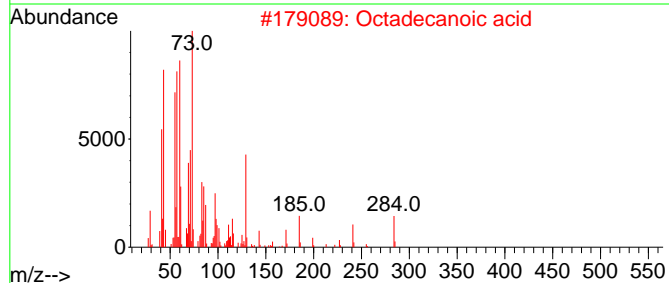
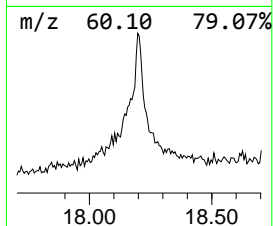
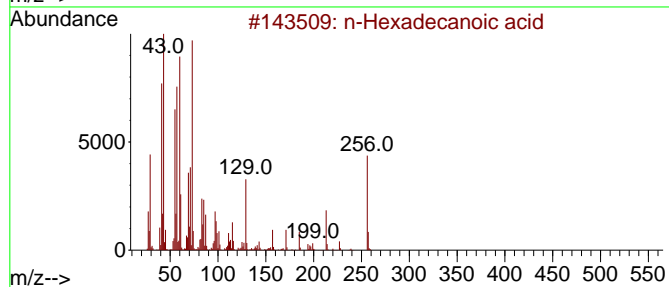
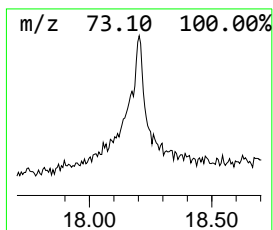
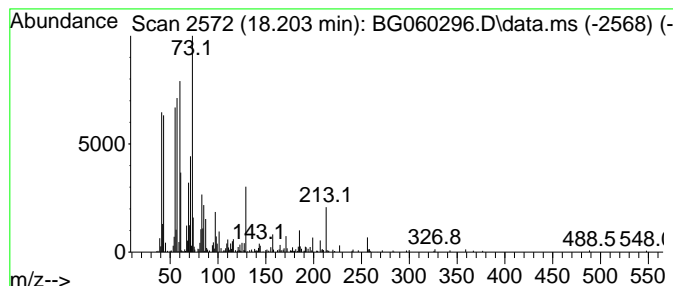
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TIC Library : C:\Database\NIST20.L
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 Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.203	7.21 ng	1207010	Phenanthrene-d10	17.316

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2		Octadecanoic acid	284	C18H36O2	000057-11-4	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	70
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5		Undecanoic acid	186	C11H22O2	000112-37-8	59



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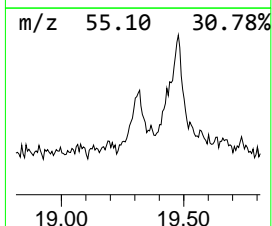
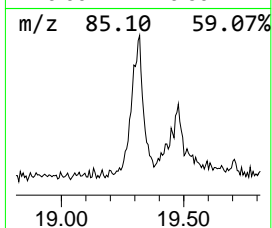
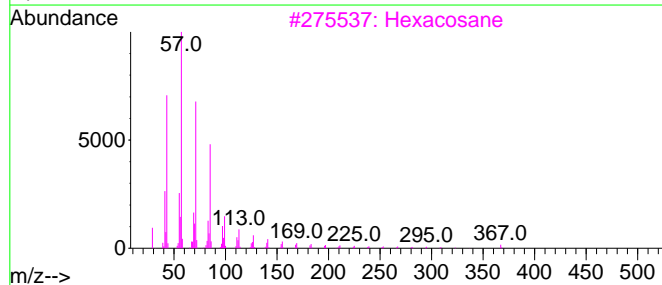
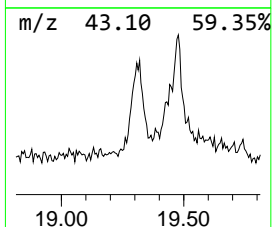
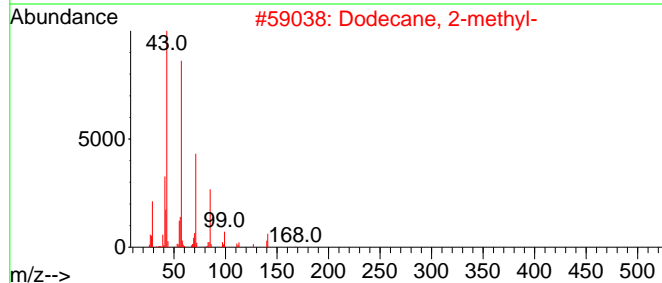
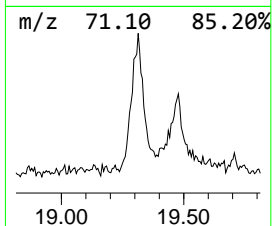
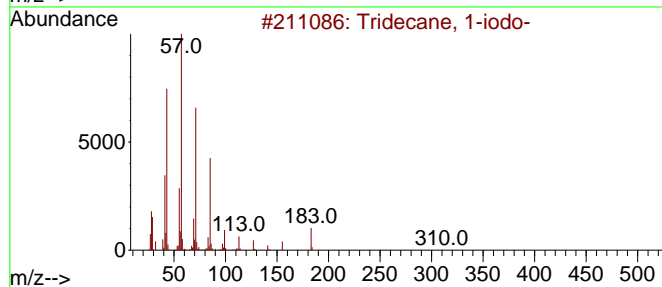
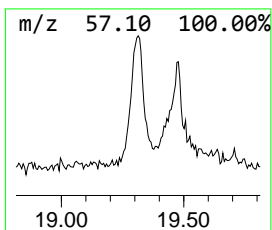
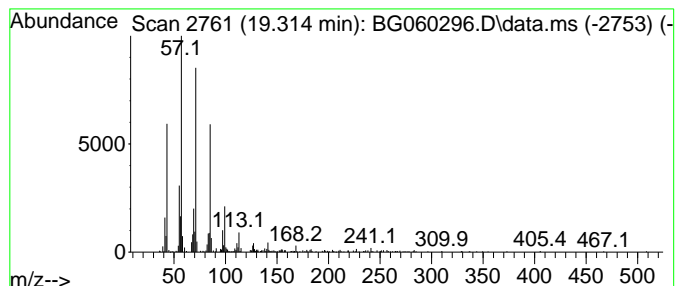
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 Peak Number 3 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.314	4.97 ng	832635	Phenanthrene-d10	17.316

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
2		Dodecane, 2-methyl-	184	C13H28	001560-97-0	83
3		Hexacosane	366	C26H54	000630-01-3	83
4		Tridecane, 7-propyl-	226	C16H34	055045-09-5	80
5		Eicosane	282	C20H42	000112-95-8	78



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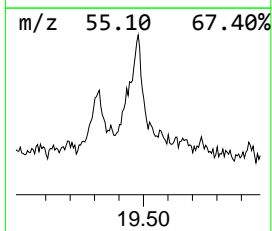
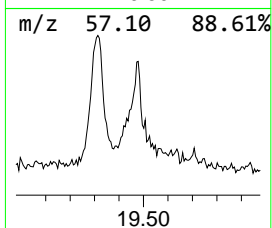
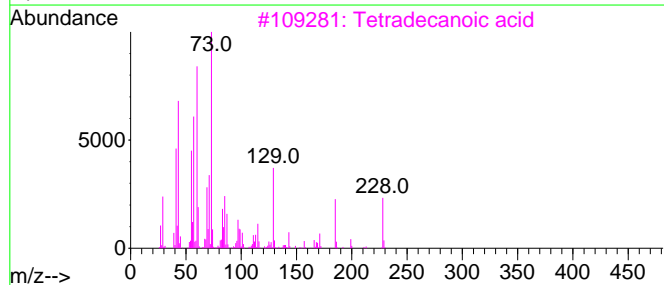
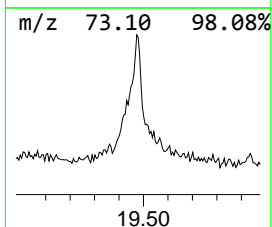
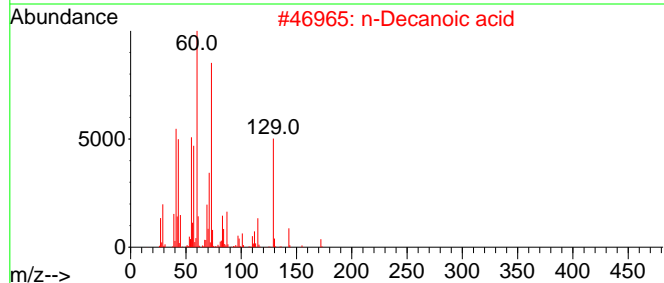
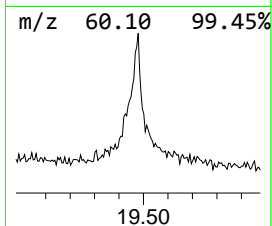
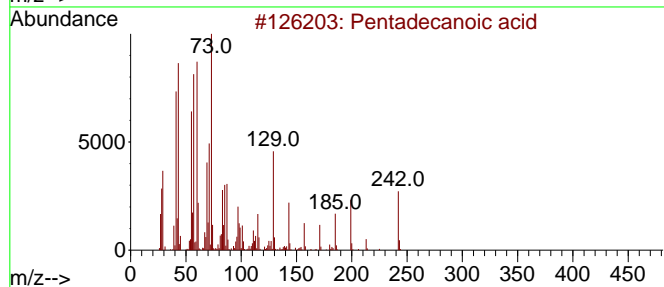
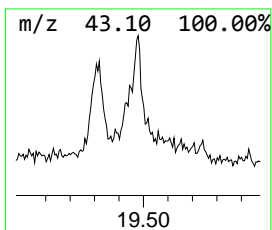
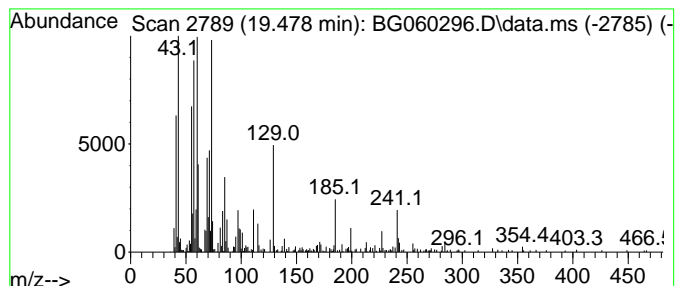
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 Peak Number 4 Pentadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.478	7.31 ng	1453150	Chrysene-d12	21.576

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
2			n-Decanoic acid	172	C10H20O2	000334-48-5	60
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4			Tridecanoic acid	214	C13H26O2	000638-53-9	50
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50



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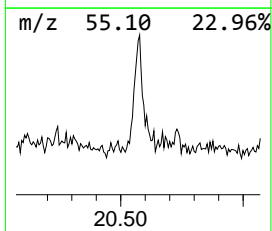
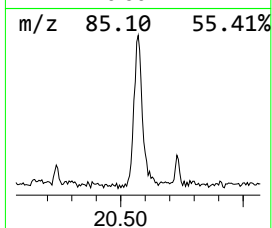
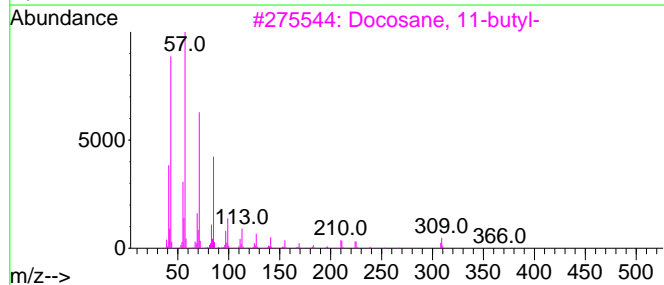
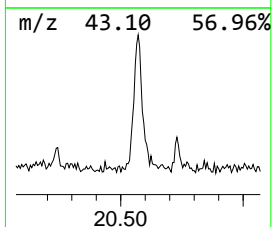
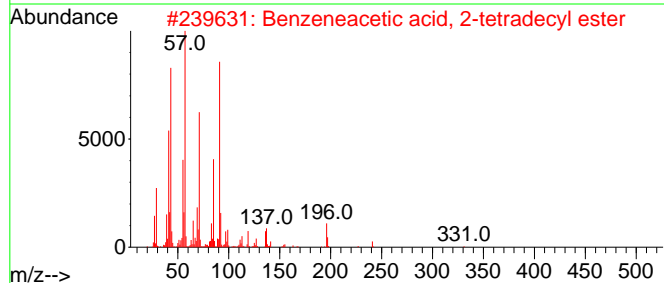
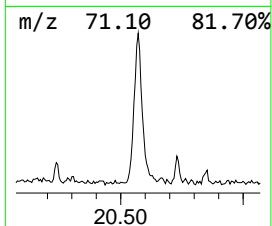
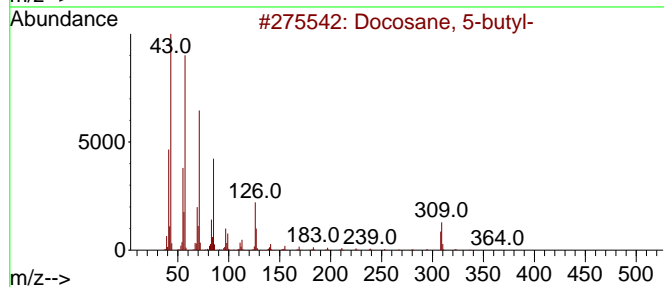
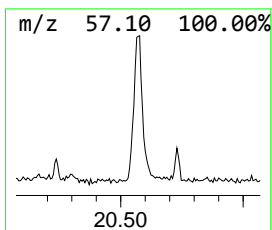
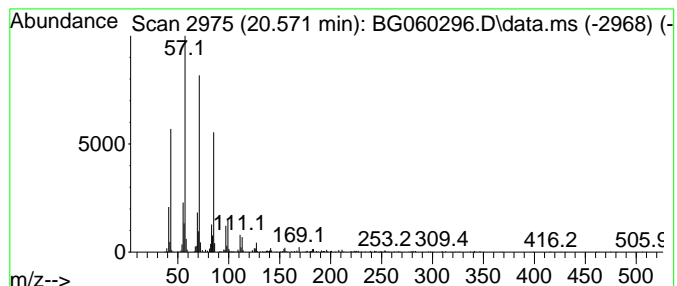
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TIC Library : C:\Database\NIST20.L
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 Peak Number 5 Docosane, 5-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.571	7.05 ng	1401000	Chrysene-d12	21.576

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 5-butyl-	366	C26H54	055282-16-1	90
2			Benzeneacetic acid, 2-tetradecyl...	332	C22H36O2	1000282-02-4	90
3			Docosane, 11-butyl-	366	C26H54	013475-76-8	86
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5			Docosane, 9-butyl-	366	C26H54	055282-14-9	86



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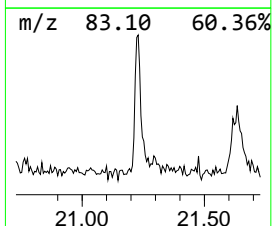
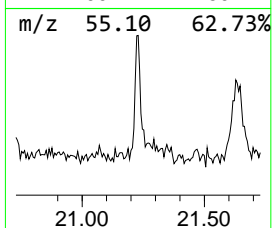
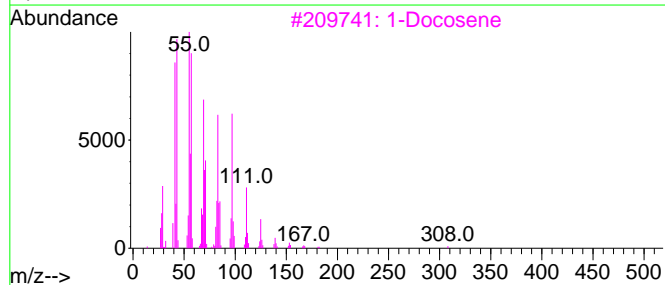
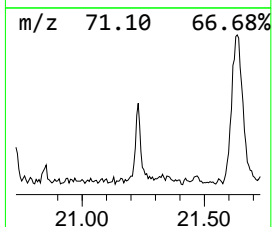
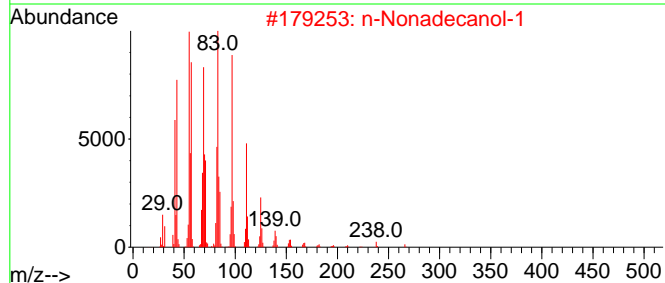
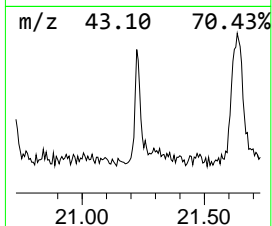
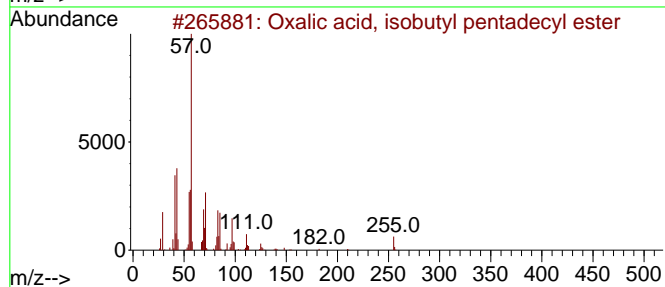
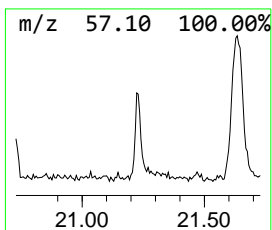
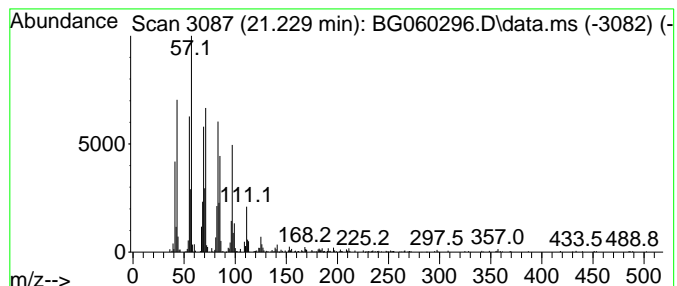
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 Oxalic acid, isobutyl penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.229	3.95 ng	784611	Chrysene-d12	21.576

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	86
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	62
3		1-Docosene	308	C22H44	001599-67-3	62
4		Behenic alcohol	326	C22H46O	000661-19-8	62
5		1-Hexacosene	364	C26H52	018835-33-1	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011024\
 Data File : BG060296.D
 Acq On : 10 Jan 2024 11:34
 Operator : MA/JU
 Sample : P1067-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SP-A-COMP(0-8)

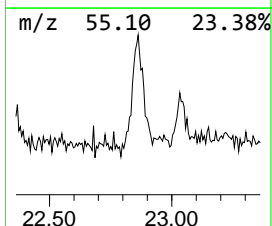
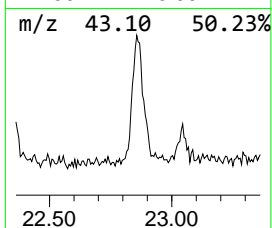
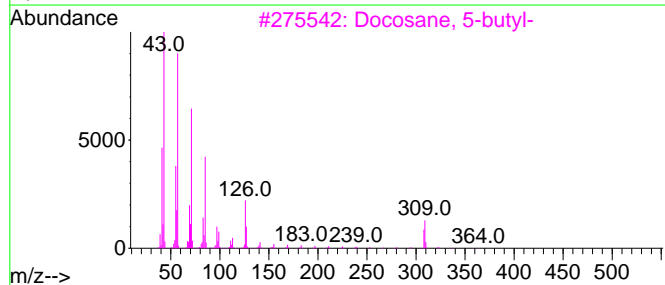
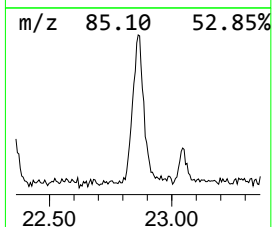
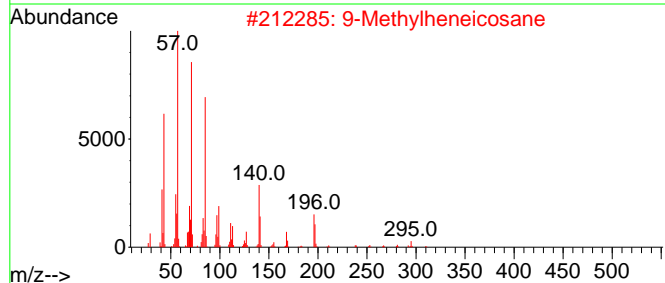
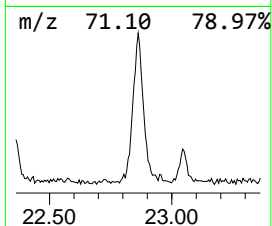
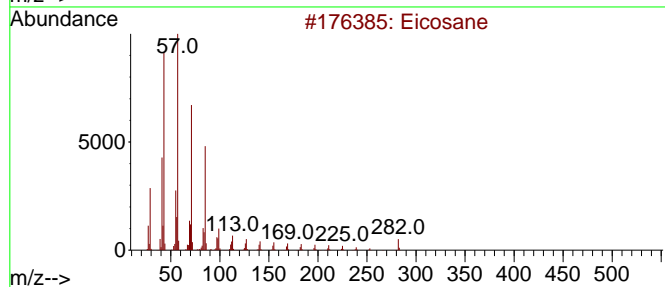
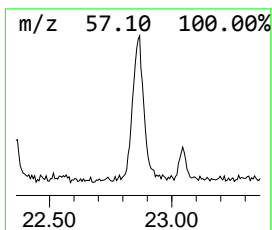
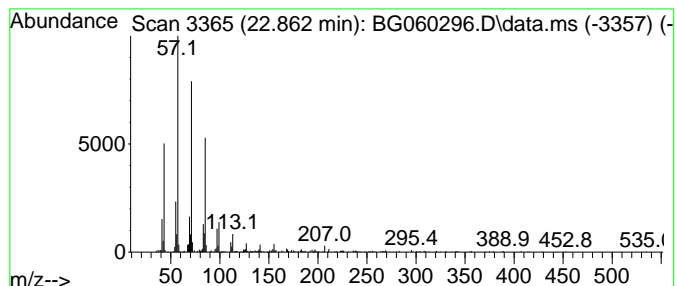
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.862	6.26 ng	1243930	Chrysene-d12	21.576

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	90
2		9-Methylheneicosane	310	C22H46	070475-51-3	87
3		Docosane, 5-butyl-	366	C26H54	055282-16-1	86
4		Nonadecane	268	C19H40	000629-92-5	86
5		Decane, 1-iodo-	268	C10H21I	002050-77-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011024\
 Data File : BG060296.D
 Acq On : 10 Jan 2024 11:34
 Operator : MA/JU
 Sample : P1067-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SP-A-COMP(0-8)

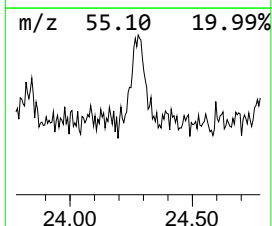
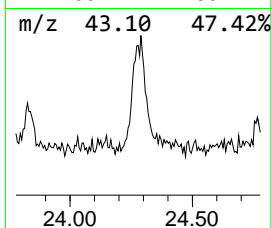
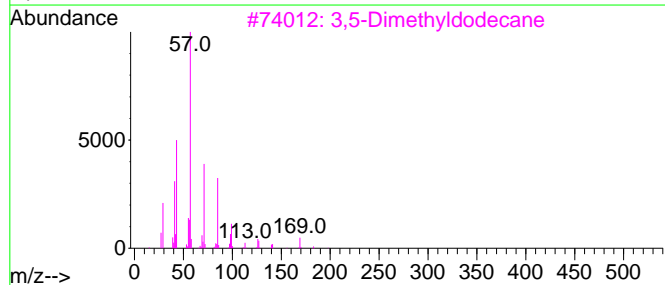
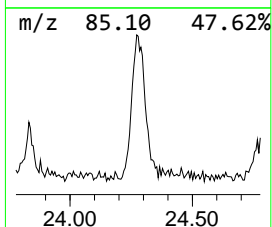
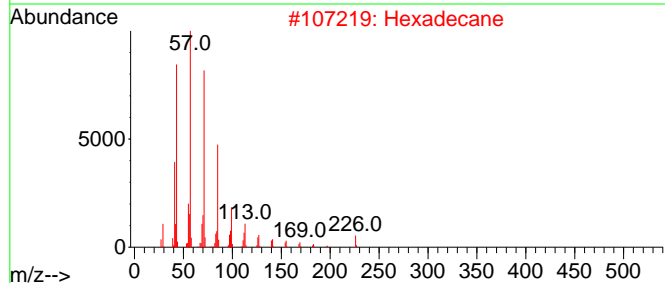
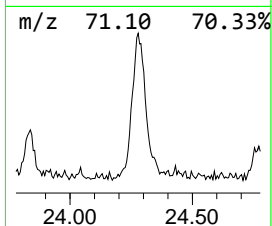
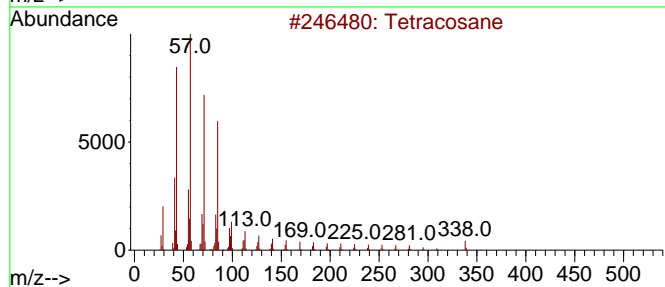
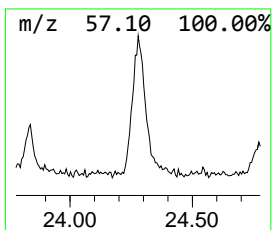
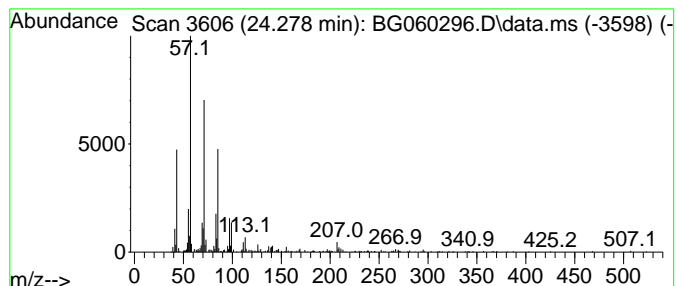
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.278	5.76 ng	1051780	Perylene-d12	24.748

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	87
2		Hexadecane	226	C16H34	000544-76-3	87
3		3,5-Dimethyldodecane	198	C14H30	107770-99-0	72
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	70
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011024\
 Data File : BG060296.D
 Acq On : 10 Jan 2024 11:34
 Operator : MA/JU
 Sample : P1067-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SP-A-COMP(0-8)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG010824.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-...	5.036	3.8	ng	237729	1	7.933	1240950	20.0
n-Hexadecanoic ...	18.203	7.2	ng	1207010	4	17.316	3350160	20.0
Tridecane, 1-iodo-	19.314	5.0	ng	832635	4	17.316	3350160	20.0
Pentadecanoic acid	19.478	7.3	ng	1453150	5	21.576	3977210	20.0
Docosane, 5-butyl-	20.571	7.0	ng	1401000	5	21.576	3977210	20.0
Oxalic acid, is...	21.229	4.0	ng	784611	5	21.576	3977210	20.0
Eicosane	22.862	6.3	ng	1243930	5	21.576	3977210	20.0
Tetracosane	24.278	5.8	ng	1051780	6	24.748	3651020	20.0