LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033545.D
Acq On : 20 Dec 2021 18:08
Operator : CG/JU
Sample : M5079-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
340

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_M\Methods\8270-BM121621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033545.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.496	39	44	64	rVB	4525470	5327000	100.00%	32.308%
2	5.025	299	304	315	rBV	357088	503081	9.44%	3.051%
3	5.490	376	383	402	rVB	778730	1154668	21.68%	7.003%
4	6.554	558	564	573	rBV	35622	61346	1.15%	0.372%
5	7.096	649	656	670	rBV	738915	1262552	23.70%	7.657%
6	7.919	787	796	806	rBV	138668	229079	4.30%	1.389%
7	9.095	988	996	1011	rBV	485118	839785	15.76%	5.093%
8	10.731	1267	1274	1285	rVB	165699	284553	5.34%	1.726%
9	13.195	1686	1693	1700	rBV	1046745	1620138	30.41%	9.826%
10	14.566	1921	1926	1933	rVB	245101	359259	6.74%	2.179%
11	16.060	2173	2180	2199	rVB	767160	1104394	20.73%	6.698%
12	17.318	2387	2394	2398	rBV	267200	394659	7.41%	2.394%
13	18.207	2539	2545	2548	rBV3	41575	70132	1.32%	0.425%
14	18.501	2590	2595	2600	rBV	47827	63317	1.19%	0.384%
15	18.989	2671	2678	2686	rBV4	20969	54955	1.03%	0.333%
16	19.065	2686	2691	2695	rVV2	52084	72398	1.36%	0.439%
17	19.130	2695	2702	2706	rVB2	38410	60025	1.13%	0.364%
18	19.936	2833	2839	2845	rBV	1501610	1889157	35.46%	11.457%
19	20.542	2938	2942	2951	rBV	55644	121544	2.28%	0.737%
20	21.195	3050	3053	3062	rVB2	84690	123520	2.32%	0.749%
21	21.495	3099	3104	3109	rBV	265536	356294	6.69%	2.161%
22	21.842	3159	3163	3174	rBV	91297	173487	3.26%	1.052%
23	23.306	3409	3412	3417	rBV	40684	66212	1.24%	0.402%
24	23.900	3507	3513	3523	rVB	144398	296857	5.57%	1.800%

Sum of corrected areas: 16488412

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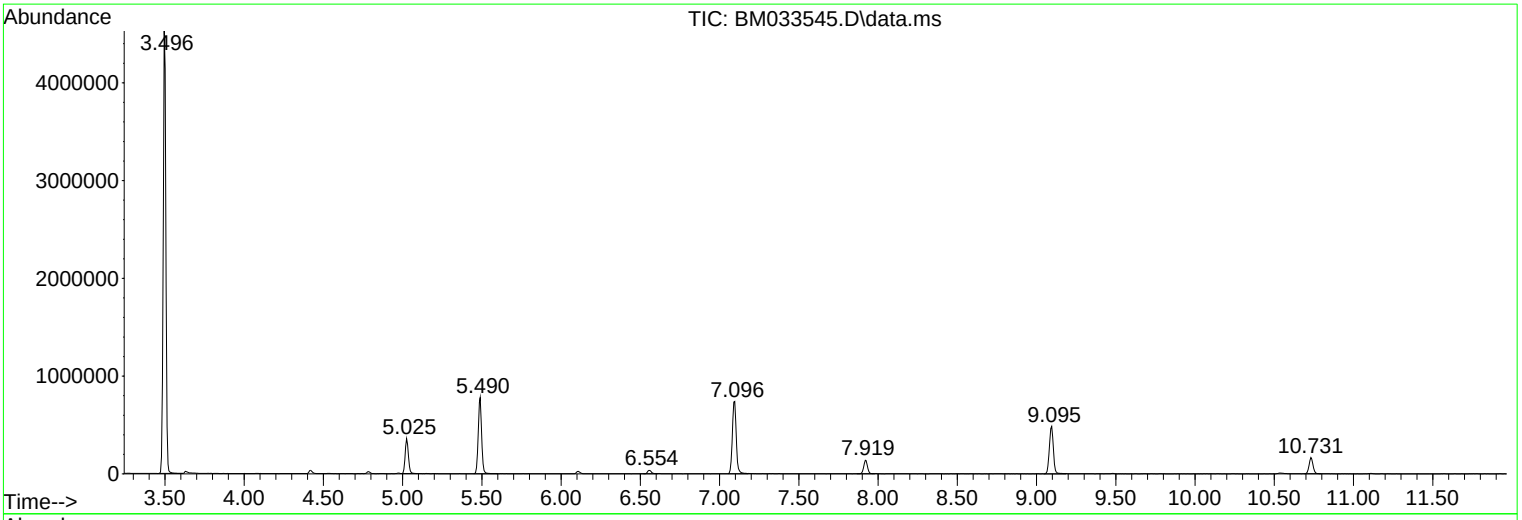
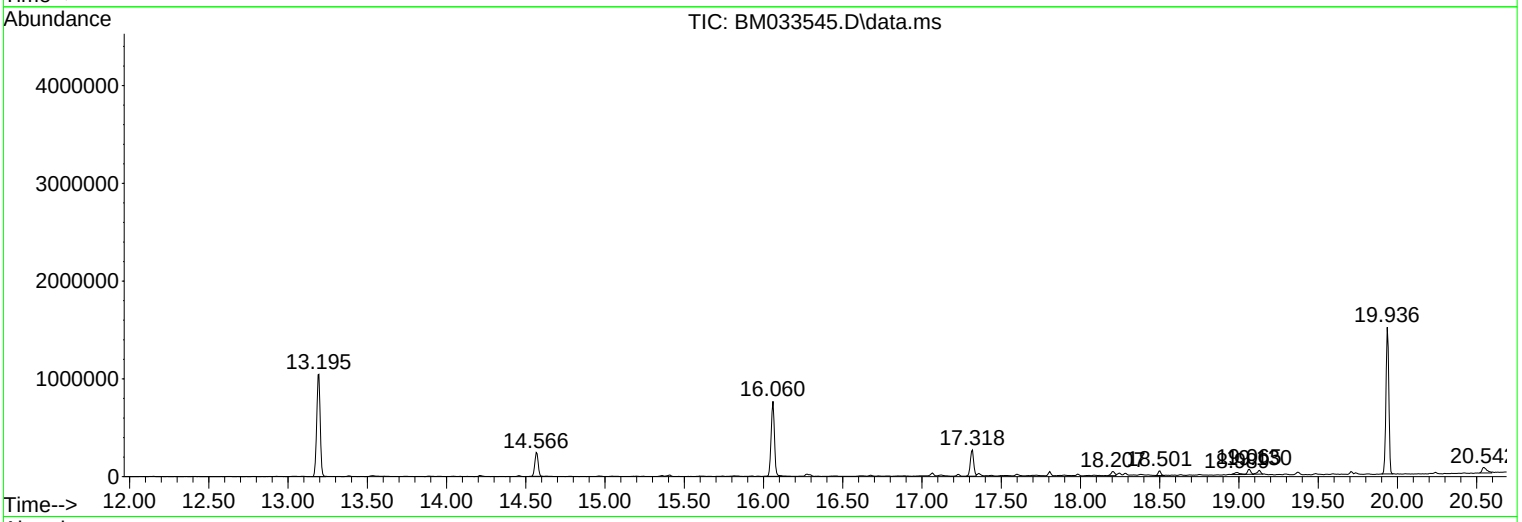
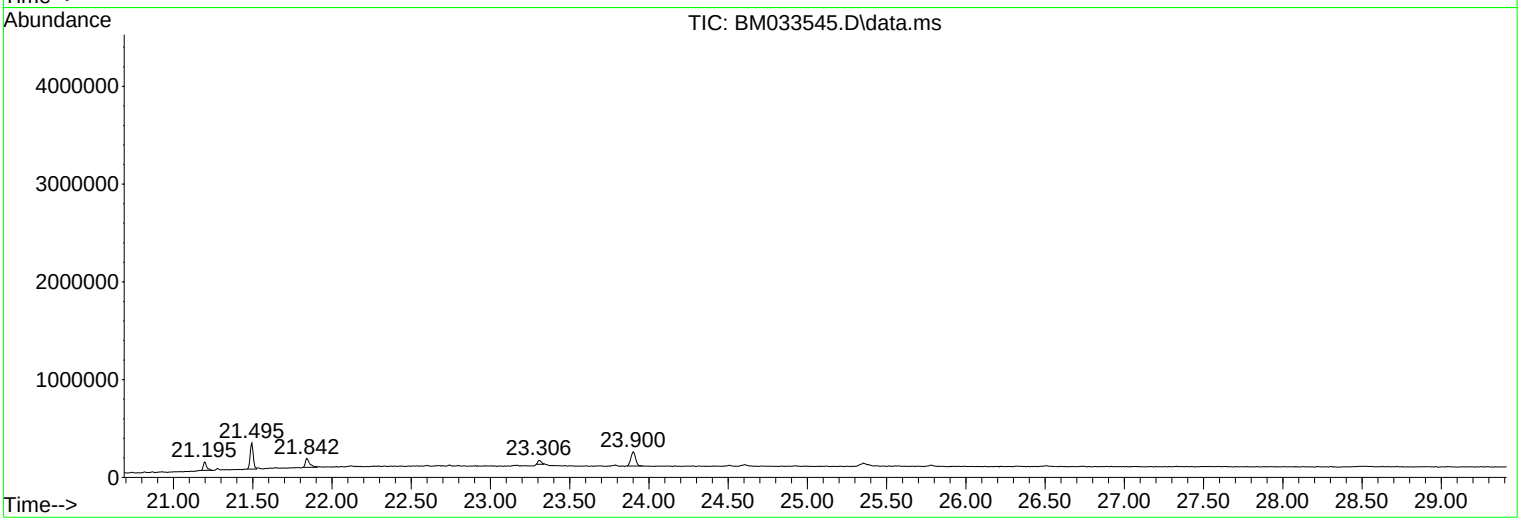
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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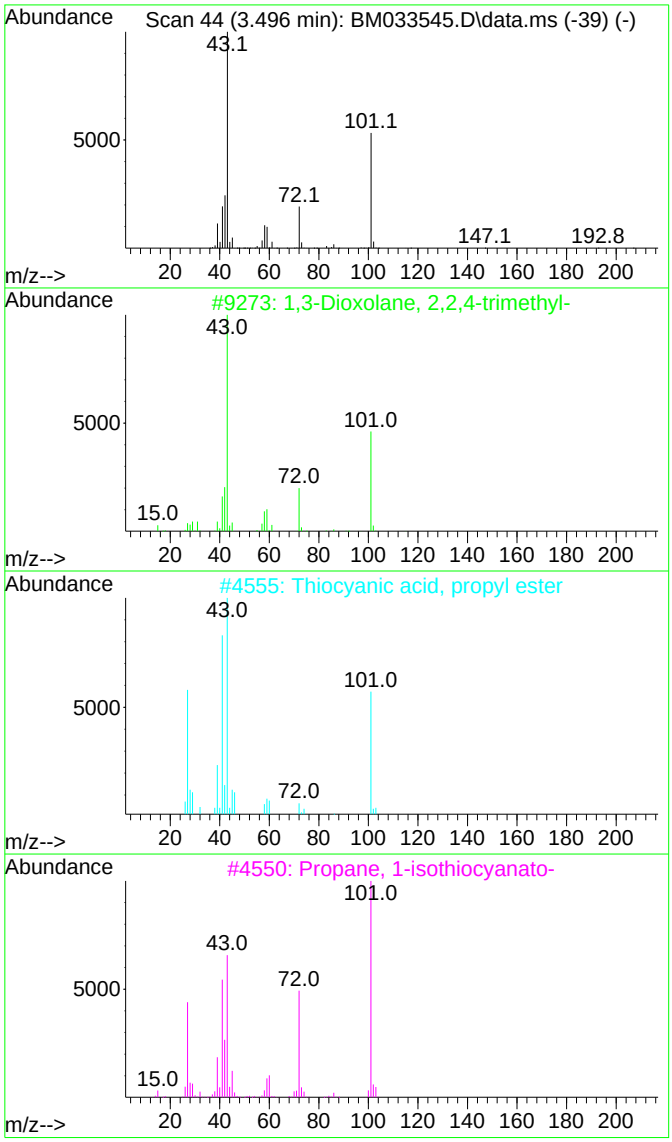
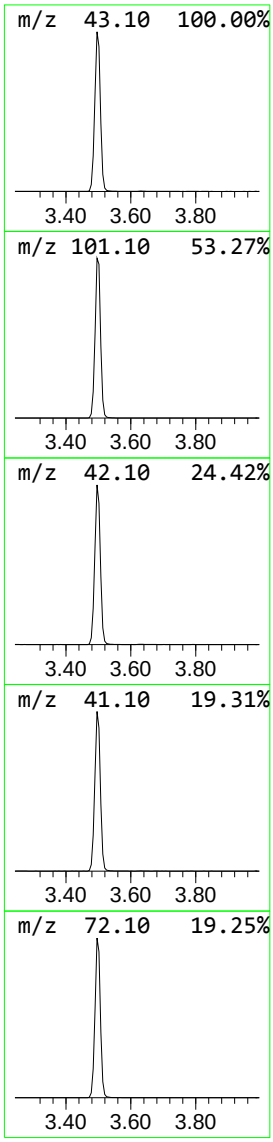
****
Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.496	465.08 ng	5327000	1,4-Dichlorobenzene-d4	7.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	53
3	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	50
4	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	50
5	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9





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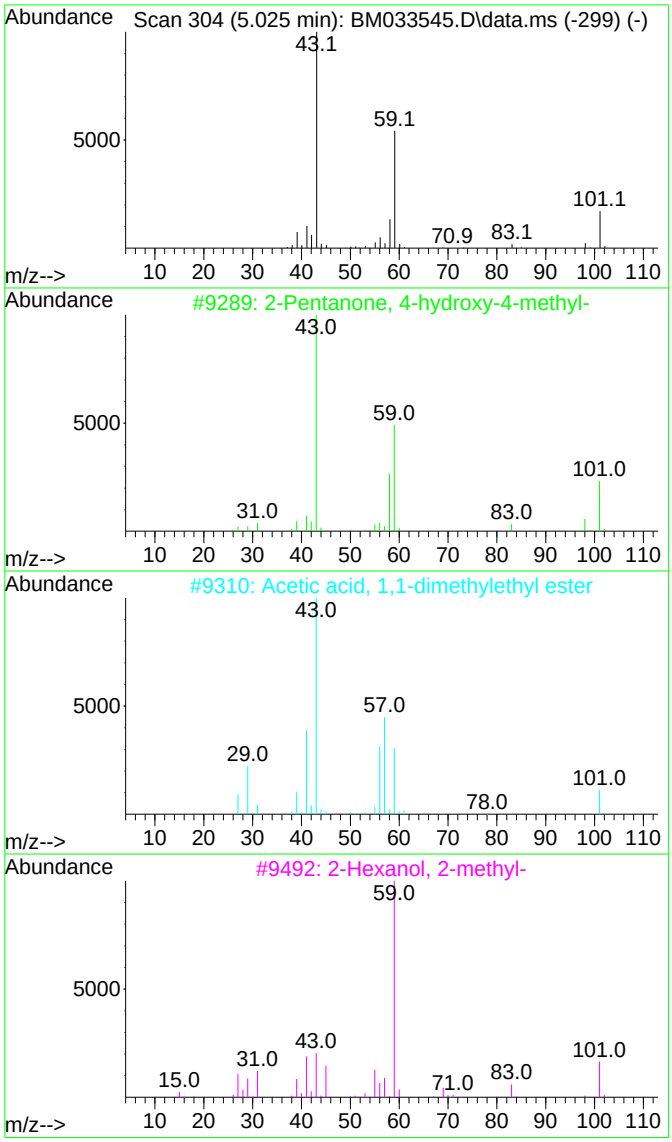
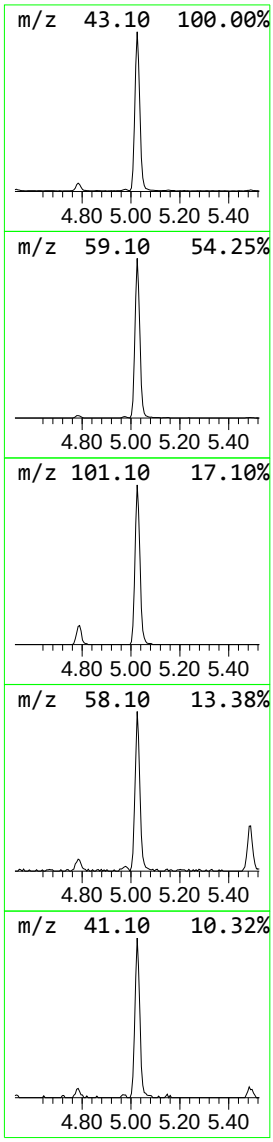
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.025	43.92 ng	503081	1,4-Dichlorobenzene-d4	7.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23





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ClientSampleId :
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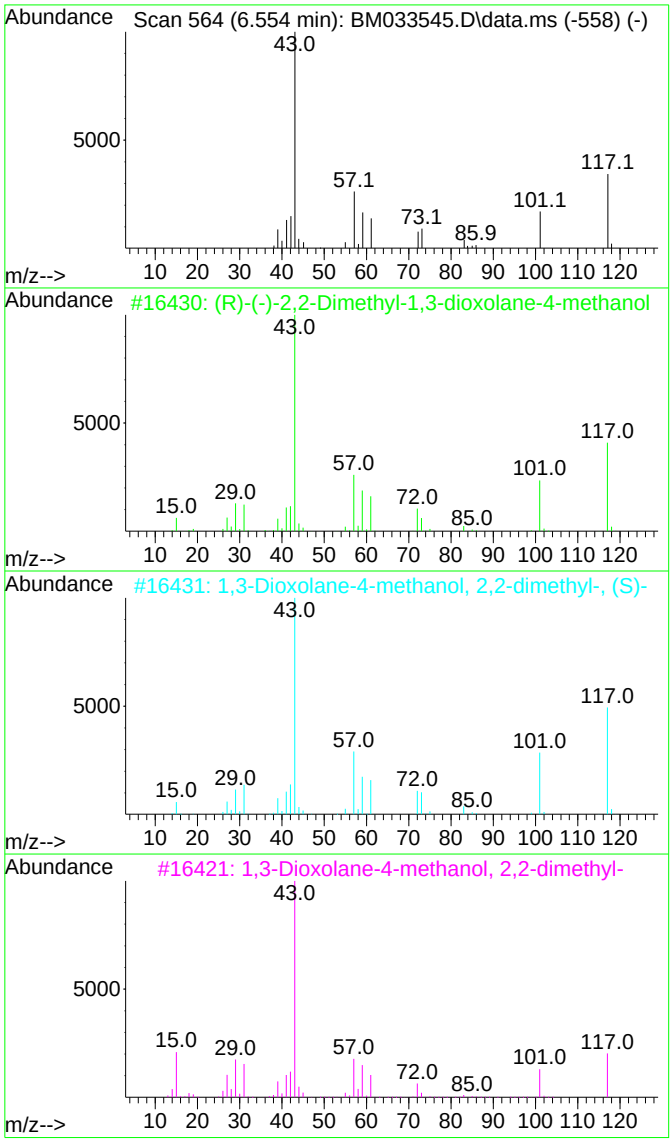
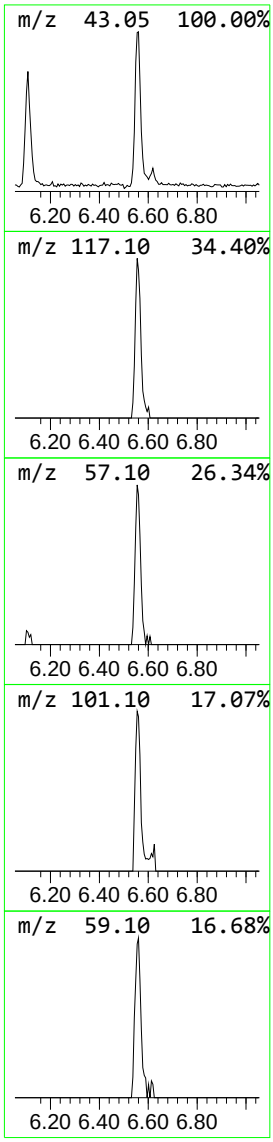
****
Peak Number 3 (R)-(-)-2,2-Dimethyl-1,3-di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.554	5.36 ng	61346	1,4-Dichlorobenzene-d4	7.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(-)-2,2-Dimethyl-1,3-dioxola...	132	C6H12O3	014347-78-5	90
2	1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	022323-82-6	90
3	1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	000100-79-8	59
4	Butanoic acid, 3-hydroxy-3-methy...	132	C6H12O3	006149-45-7	33
5	3-Ethoxypropyl acetate	146	C7H14O3	1000378-33-4	28





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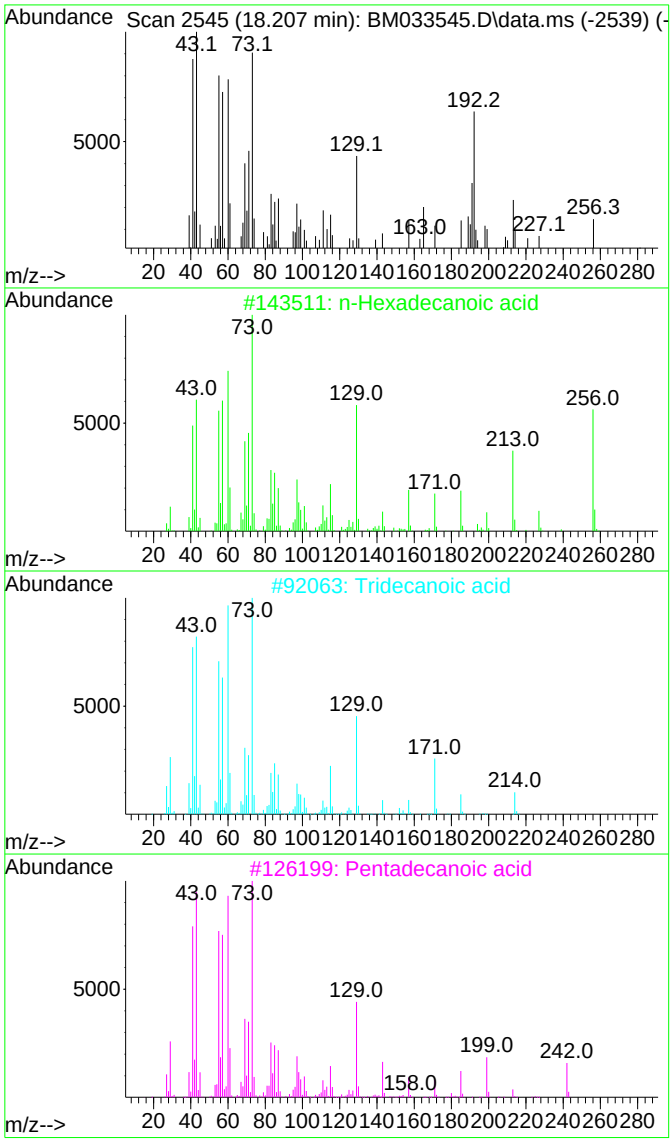
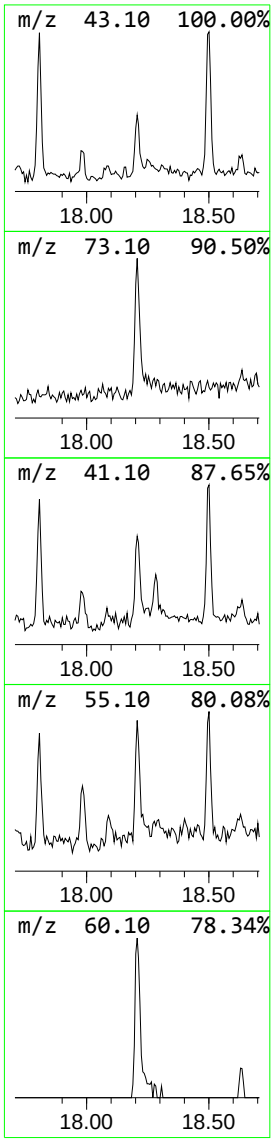
Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.207	3.55 ng	70132	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	25





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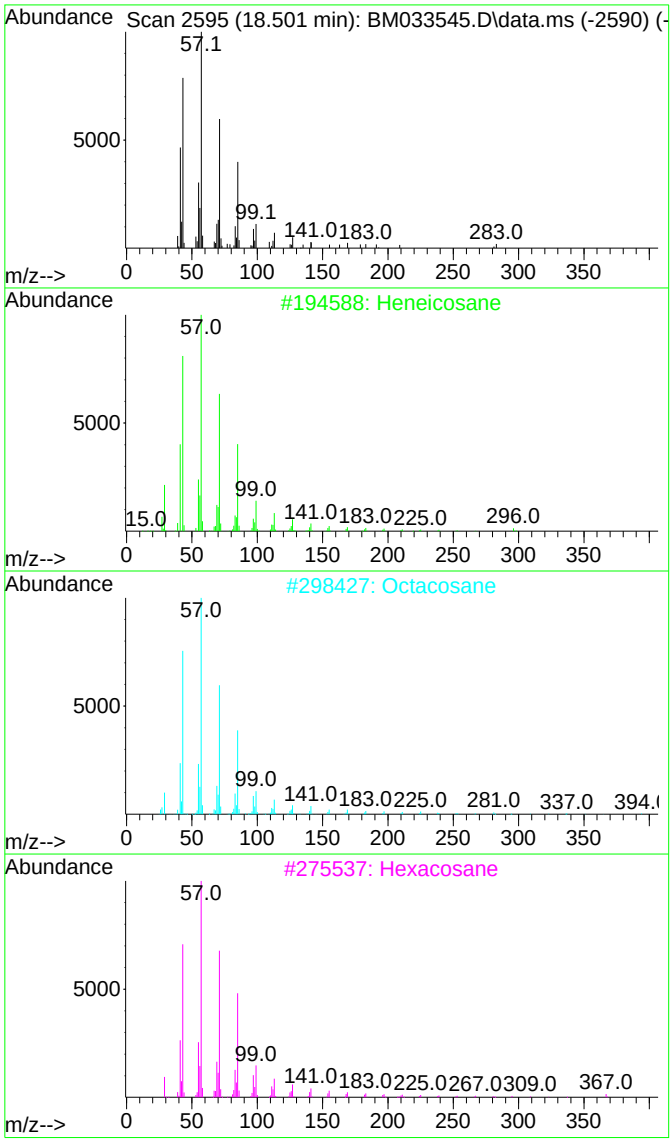
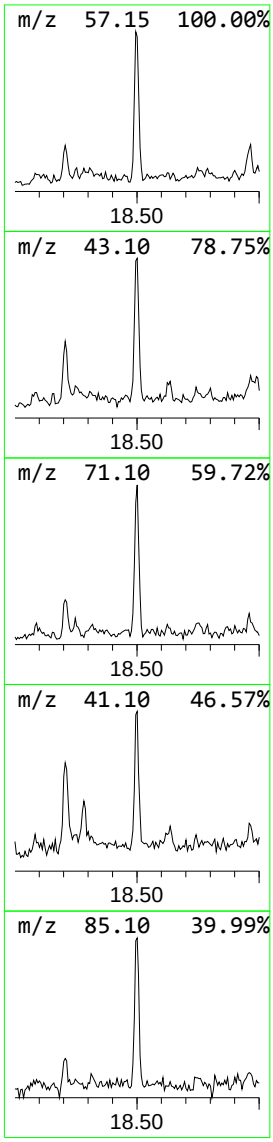
Peak Number 5 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.501	3.21 ng	63317	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Tetracosane	338	C24H50	000646-31-1	91





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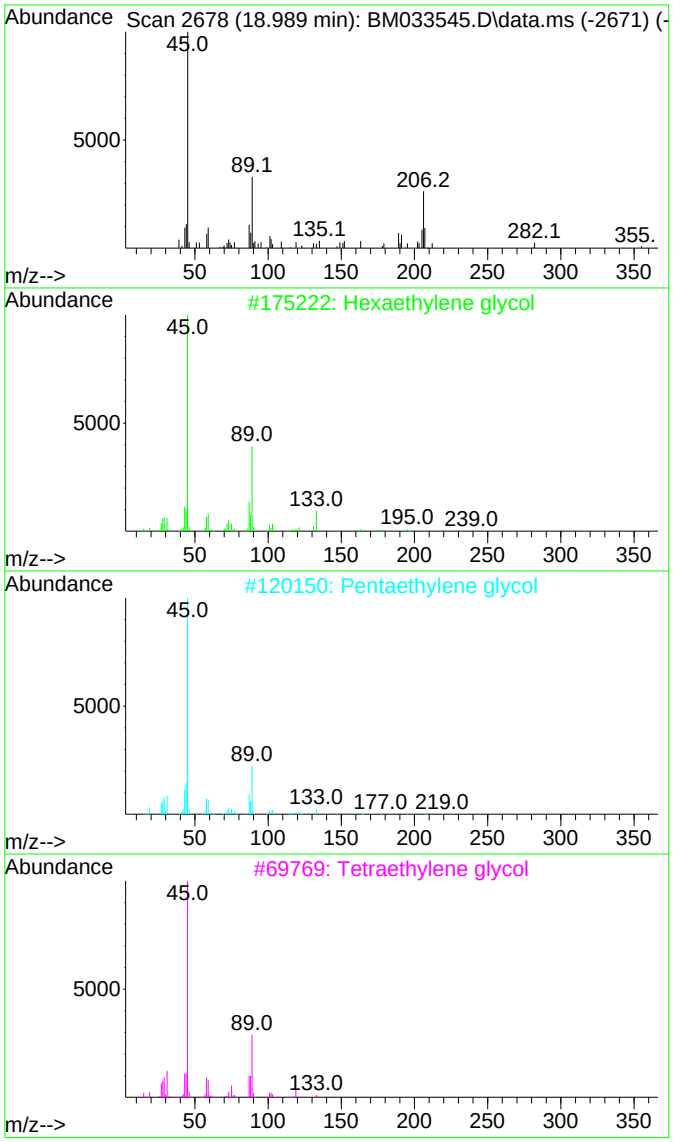
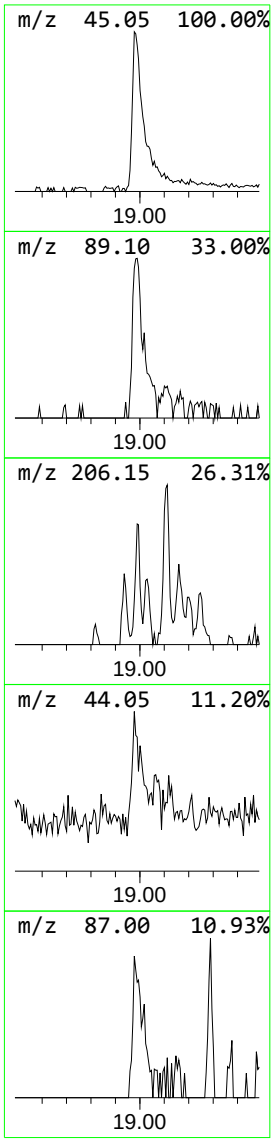
****

Peak Number 6 Hexaethylene glycol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.989	2.78 ng	54955	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	53
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	53
3	Tetraethylene glycol	194	C8H18O5	000112-60-7	53
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
5	Tetraethyleneglycol monomethylether	208	C9H20O5	023783-42-8	50





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TIC Library : C:\Database\NIST20.L
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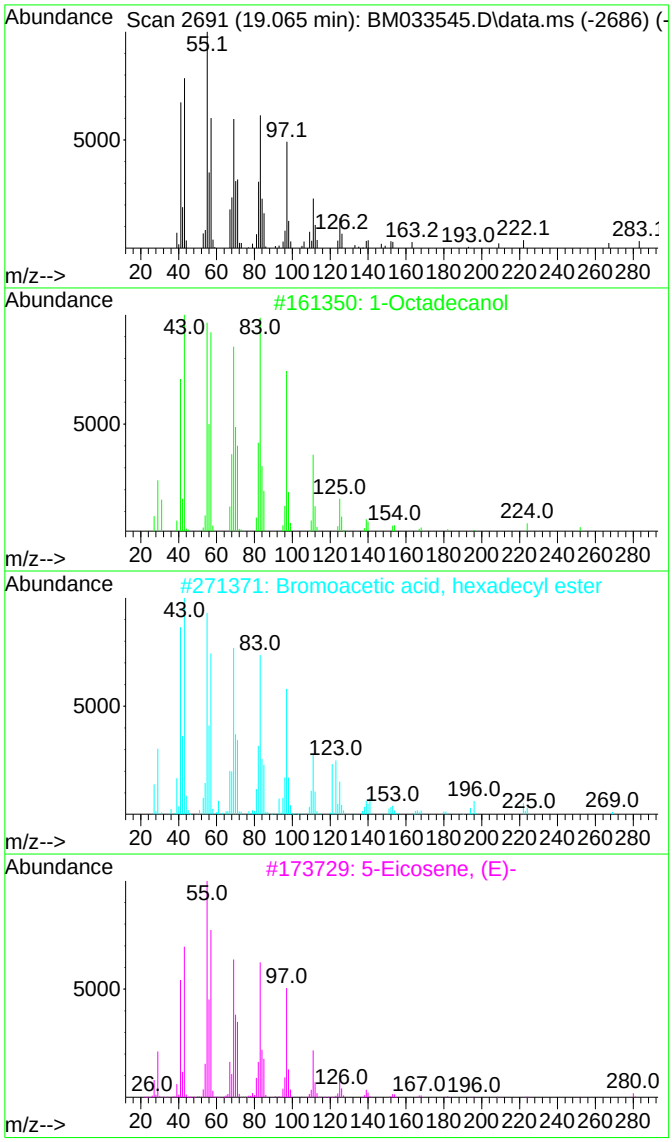
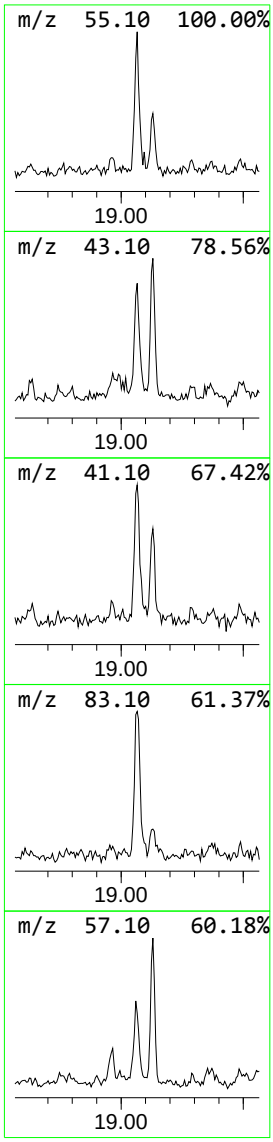
****

Peak Number 7 1-Octadecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.065	3.67 ng	72398	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	95
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91





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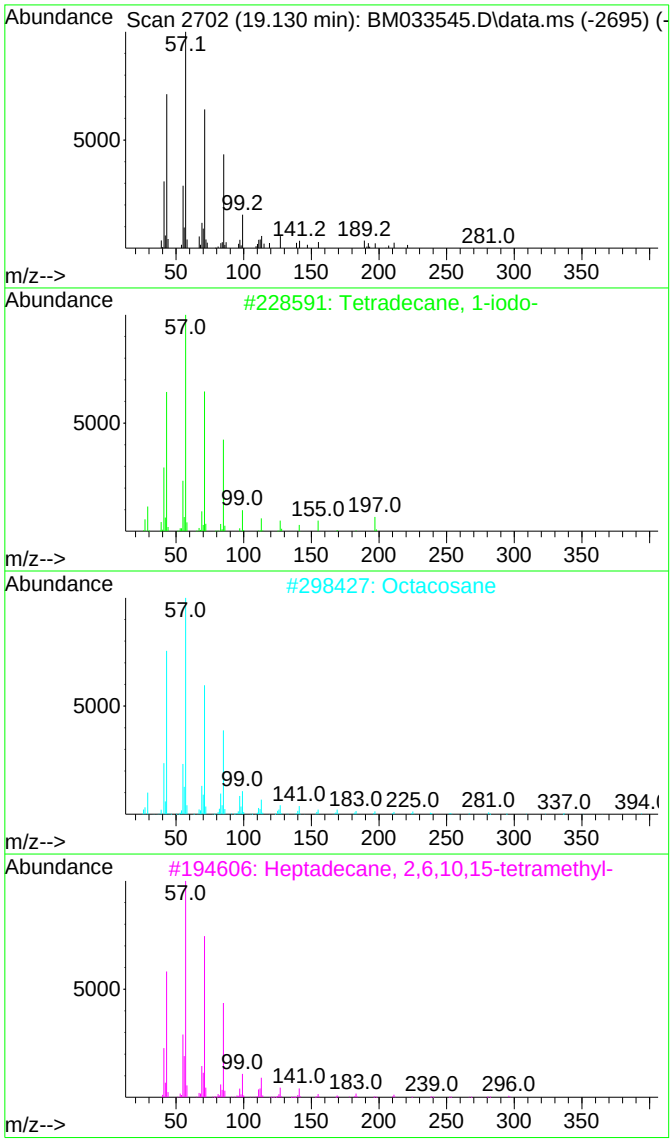
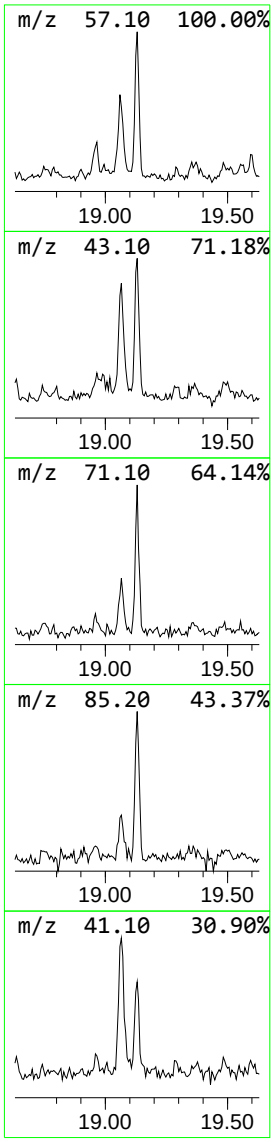
Peak Number 8 Tetradecane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.130	3.04 ng	60025	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
2	Octacosane	394	C28H58	000630-02-4	86
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
4	Heptadecane	240	C17H36	000629-78-7	83
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





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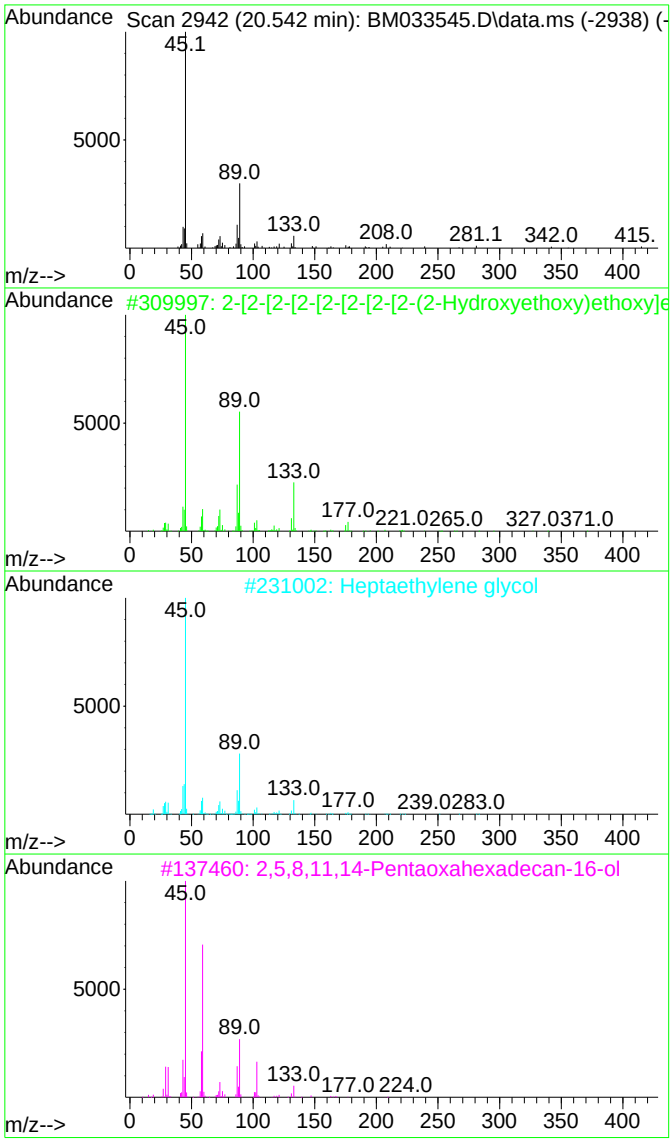
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

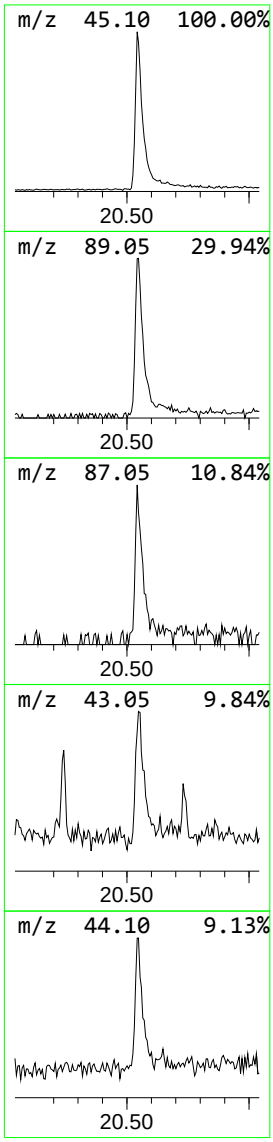
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2-[2-[2-[2-[2-[2-[2-[2-(2-H... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.542	6.82 ng	121544	Chrysene-d12	21.495

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	90
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	86
3	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	86
4	Triethylene glycol	150	C6H14O4	000112-27-6	64
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	64





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ClientSampleId :
340

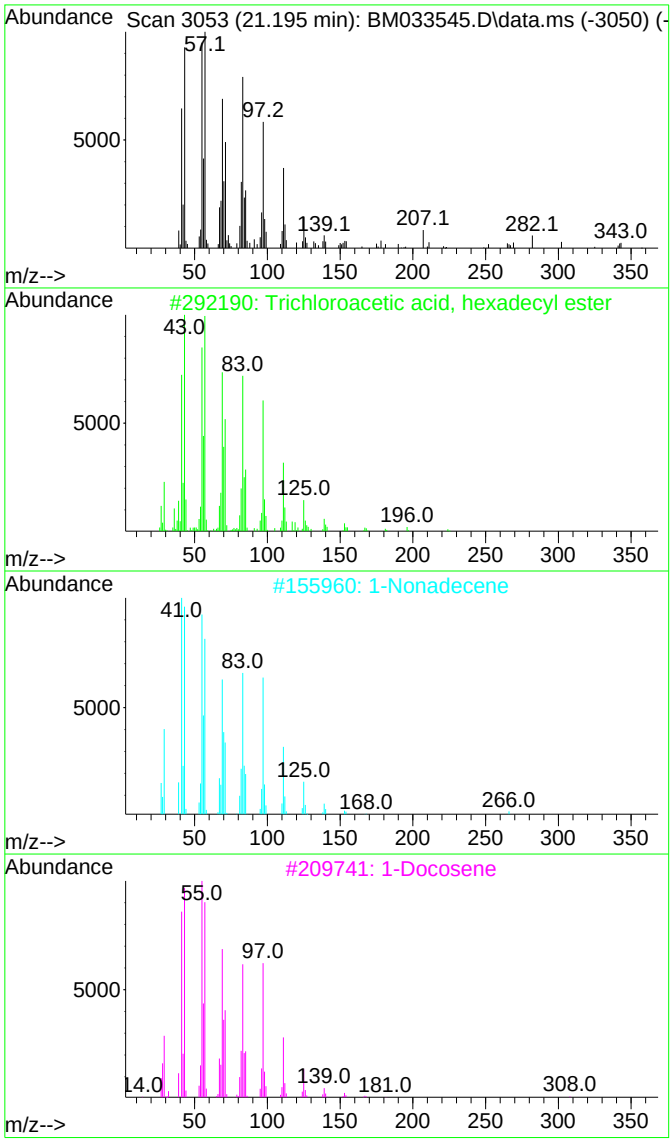
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

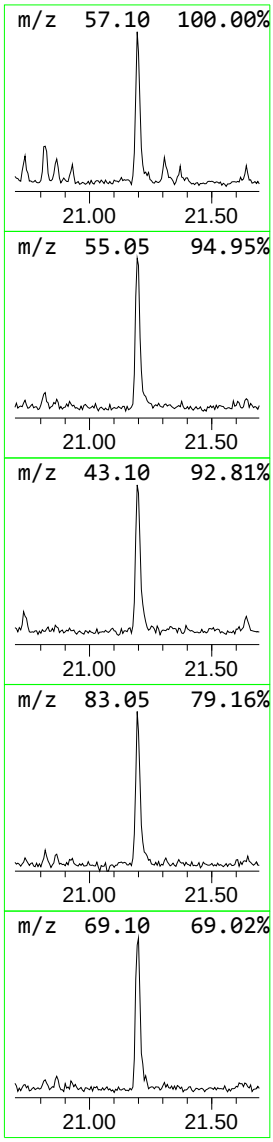
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.195	6.93 ng	123520	Chrysene-d12	21.495

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2	1-Nonadecene	266	C19H38	018435-45-5	95
3	1-Docosene	308	C22H44	001599-67-3	95
4	Octacosanol	410	C28H58O	000557-61-9	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033545.D
Acq On : 20 Dec 2021 18:08
Operator : CG/JU
Sample : M5079-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
340

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

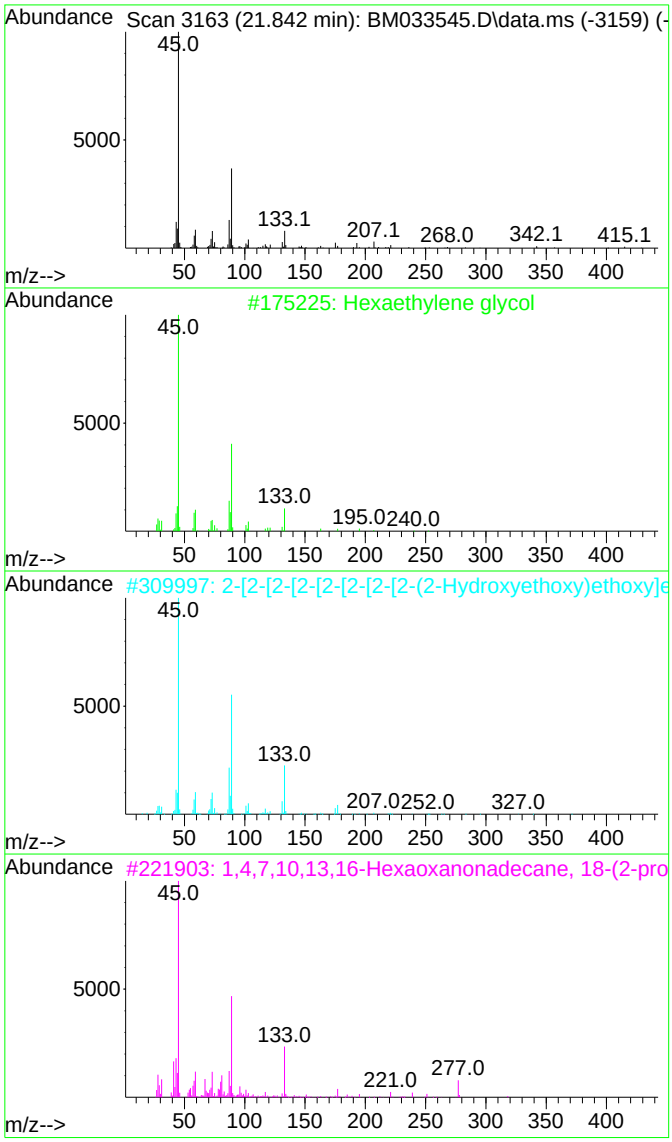
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

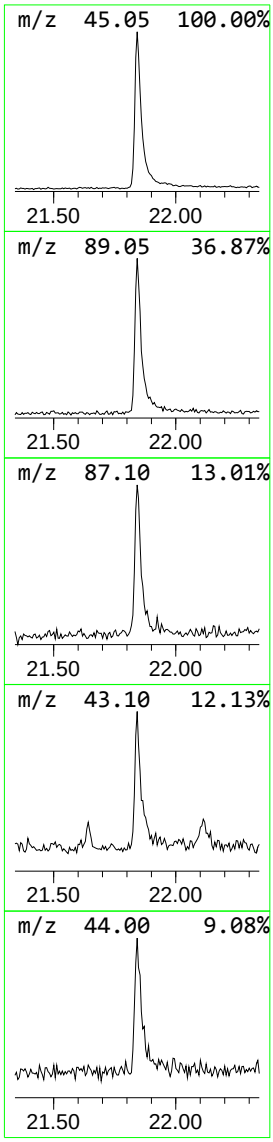
****

Peak Number 11 1,4,7,10,13,16-Hexaoxanonad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.842	9.74 ng	173487	Chrysene-d12	21.495

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	91
2	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	90
3	1,4,7,10,13,16-Hexaoxanonadecane...	318	C16H30O6	1000163-64-0	83
4	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	72
5	2-[2-[2-[2-[2-[2-[2-(2-Methoxyet...	384	C17H36O9	025990-96-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033545.D
Acq On : 20 Dec 2021 18:08
Operator : CG/JU
Sample : M5079-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
340

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

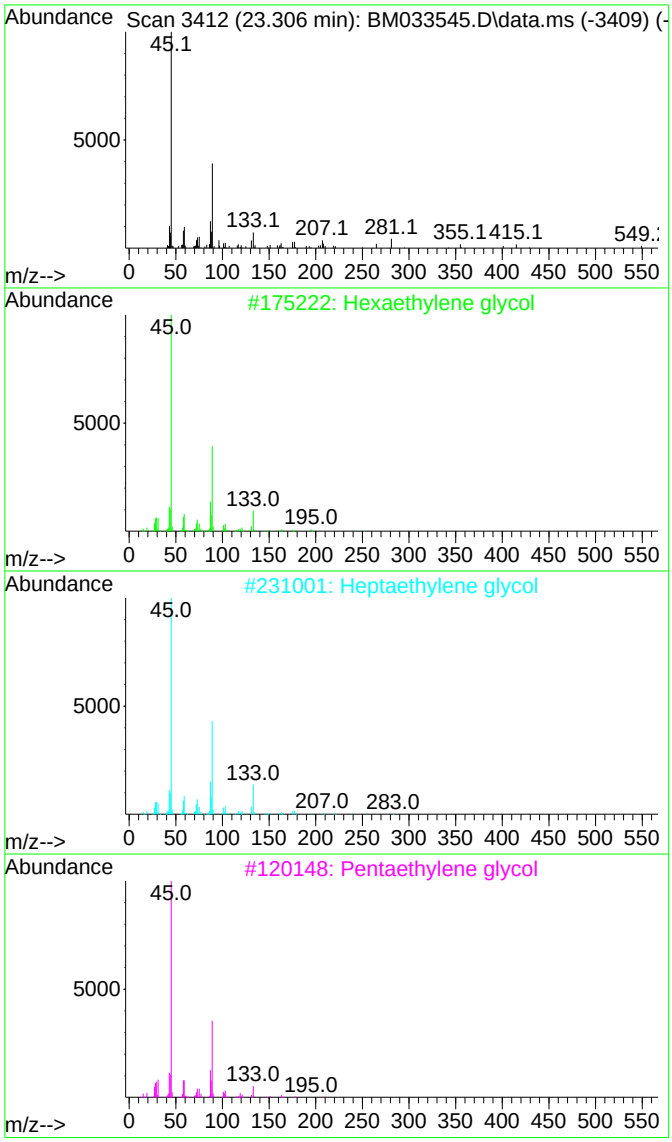
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

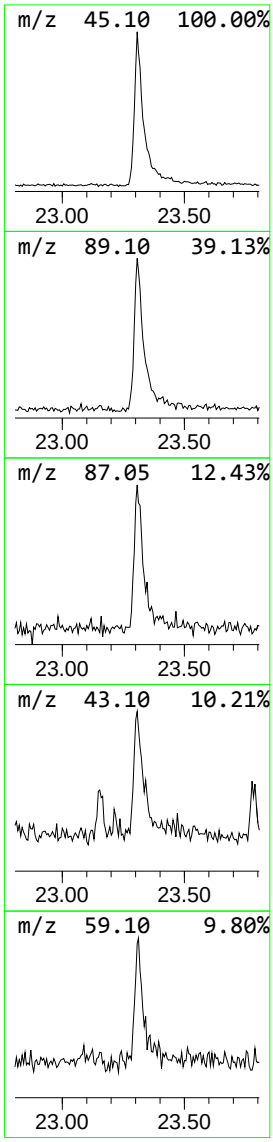
****

Peak Number 12 Heptaethylene glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.306	4.46 ng	66212	Perylene-d12	23.900

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	80
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	72
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	72
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	72
5	n-Octylpentaoxyethylene	350	C18H38O6	019327-40-3	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
Data File : BM033545.D
Acq On : 20 Dec 2021 18:08
Operator : CG/JU
Sample : M5079-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
340

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1,3-Dioxolane, ...	3.496	465.1	ng	5327000	1	7.919	229079	20.0
2-Pentanone, 4-...	5.025	43.9	ng	503081	1	7.919	229079	20.0
(R)-(-)-2,2-Dim...	6.554	5.4	ng	61346	1	7.919	229079	20.0
n-Hexadecanoic ...	18.207	3.5	ng	70132	4	17.318	394659	20.0
Heneicosane	18.501	3.2	ng	63317	4	17.318	394659	20.0
Hexaethylene gl...	18.989	2.8	ng	54955	4	17.318	394659	20.0
1-Octadecanol	19.065	3.7	ng	72398	4	17.318	394659	20.0
Tetradecane, 1-...	19.130	3.0	ng	60025	4	17.318	394659	20.0
2-[2-[2-[2-[2-[...	20.542	6.8	ng	121544	5	21.495	356294	20.0
Trichloroacetic...	21.195	6.9	ng	123520	5	21.495	356294	20.0
1,4,7,10,13,16-...	21.842	9.7	ng	173487	5	21.495	356294	20.0
Heptaethylene g...	23.306	4.5	ng	66212	6	23.900	296857	20.0