LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054331.D
Acq On : 20 Jul 2022 17:22
Operator : CG/JU
Sample : N3767-07 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-P

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054331.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.568	365	371	379	rVB	51701	92857	1.54%	0.848%
2	7.166	637	643	653	rVB	54826	107210	1.78%	0.979%
3	7.995	778	784	791	rVB	62947	104455	1.73%	0.954%
4	9.158	975	982	992	rVB	44030	83940	1.39%	0.767%
5	10.145	1133	1150	1153	rBV4	25826	84045	1.40%	0.768%
6	10.186	1153	1157	1177	rVB3	29652	75082	1.25%	0.686%
7	10.803	1255	1262	1270	rVB	80339	150161	2.49%	1.372%
8	11.638	1397	1404	1413	rBV3	31595	75396	1.25%	0.689%
9	12.936	1616	1625	1638	rBV2	30155	66585	1.11%	0.608%
10	13.248	1669	1678	1685	rBV	145087	232446	3.86%	2.123%
11	14.628	1906	1913	1919	rBV	152504	253176	4.21%	2.313%
12	15.057	1979	1986	1995	rBV3	59212	100895	1.68%	0.922%
13	16.115	2160	2166	2172	rBV2	142977	227127	3.77%	2.075%
14	16.203	2176	2181	2188	rBV	172907	262736	4.36%	2.400%
15	16.273	2188	2193	2199	rVV3	40975	63516	1.05%	0.580%
16	16.773	2273	2278	2287	rBV3	41623	68464	1.14%	0.625%
17	17.372	2370	2380	2390	rBV	249000	448102	7.44%	4.093%
18	18.271	2526	2533	2542	rBV2	183571	305016	5.07%	2.786%
19	19.188	2683	2689	2693	rBV3	36028	74182	1.23%	0.678%
20	19.417	2724	2728	2740	rBV4	64148	148198	2.46%	1.354%
21	19.540	2744	2749	2759	rVV	248374	358024	5.95%	3.270%
22	19.981	2820	2824	2830	rVB	328187	439354	7.30%	4.013%
23	20.486	2907	2910	2913	rBV4	42834	66168	1.10%	0.604%
24	20.527	2913	2917	2923	rVB2	133267	202243	3.36%	1.847%
25	20.662	2928	2940	2953	rVV	2547431	6020668	100.00%	54.995%
26	21.644	3102	3107	3119	rVB	238414	420074	6.98%	3.837%
27	24.852	3648	3653	3666	rVB2	153461	417451	6.93%	3.813%

Sum of corrected areas: 10947571

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Instrument :
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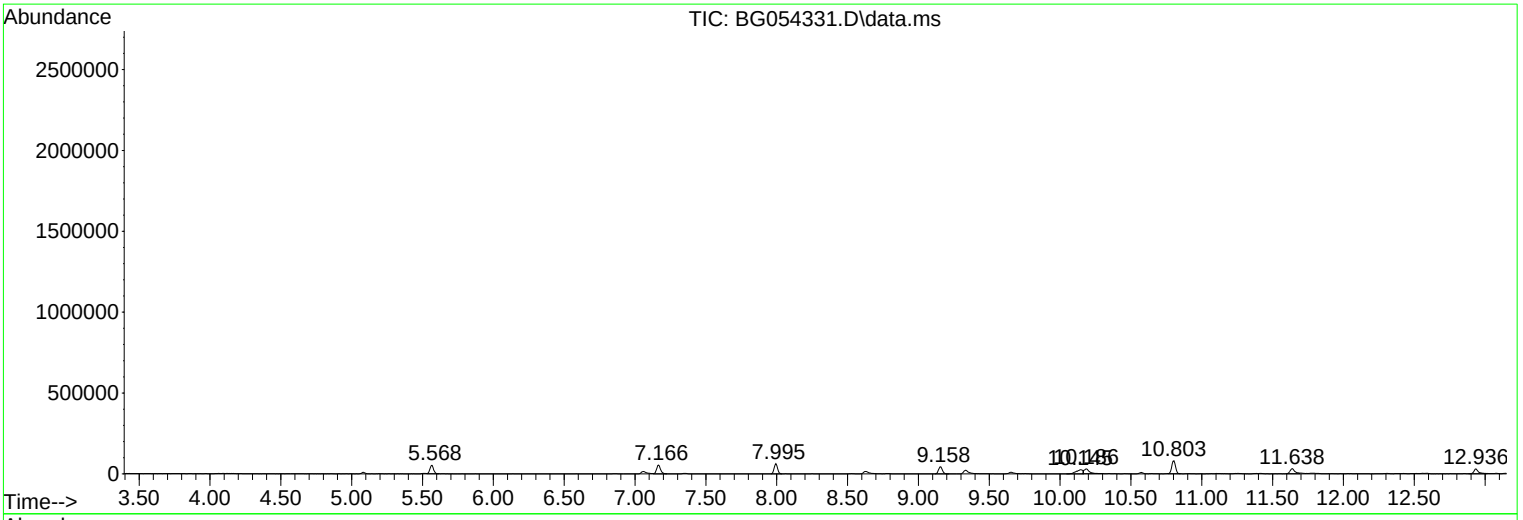
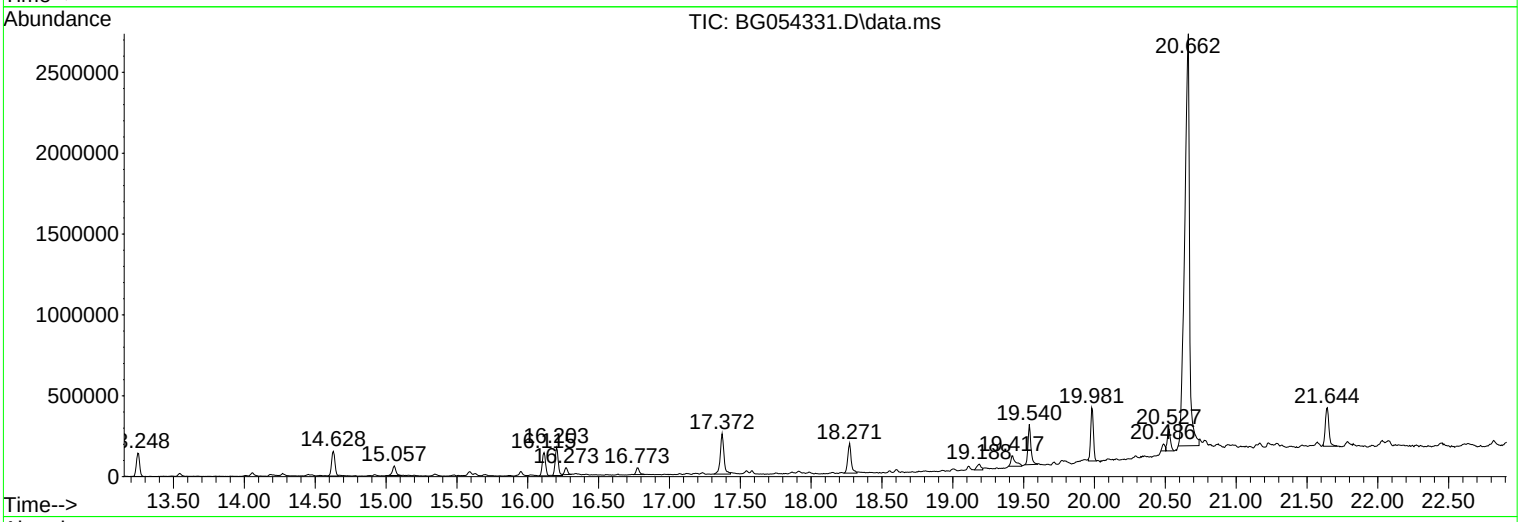
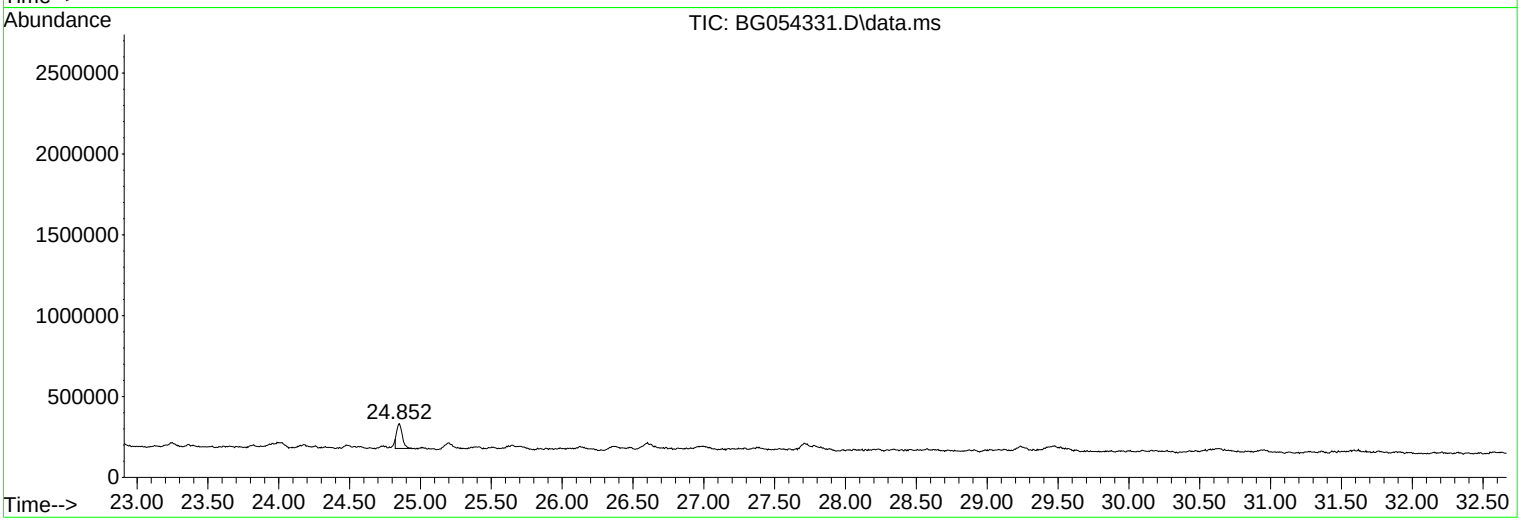
ClientSampleId :
TANK-P

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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TIC Library : C:\Database\NIST20.L
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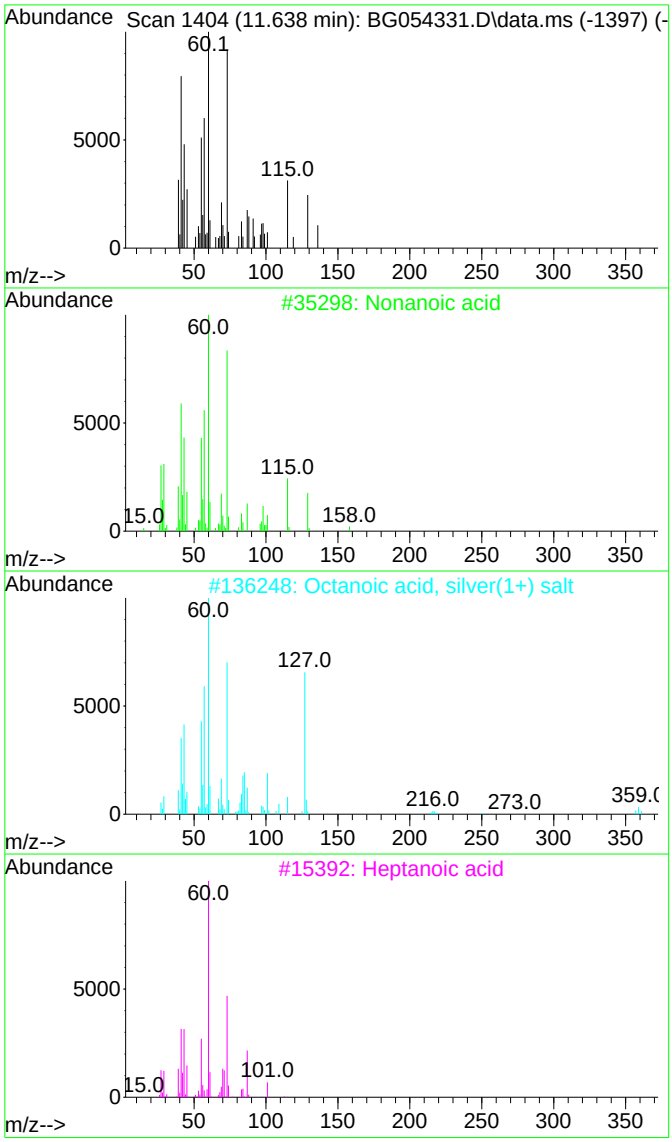
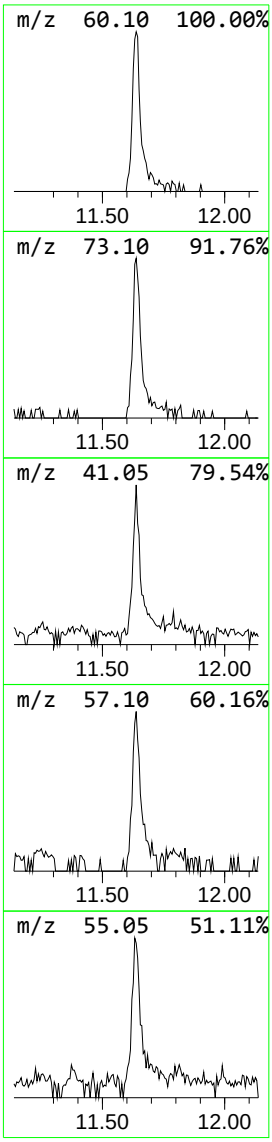
****

Peak Number 1 Nonanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.638	10.04 ng	75396	Naphthalene-d8	10.803

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	80
2	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	47
3	Heptanoic acid	130	C7H14O2	000111-14-8	38
4	1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	38
5	Hexanoic acid	116	C6H12O2	000142-62-1	37





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Data File : BG054331.D
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Operator : CG/JU
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Misc :
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Instrument :
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ClientSampleId :
TANK-P

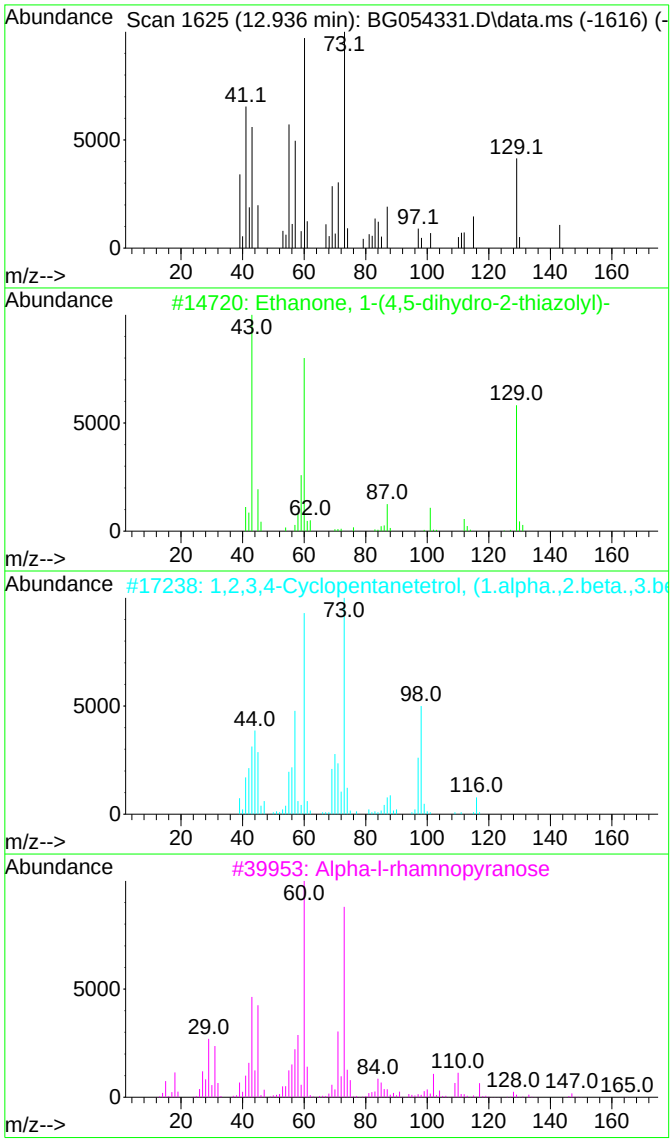
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

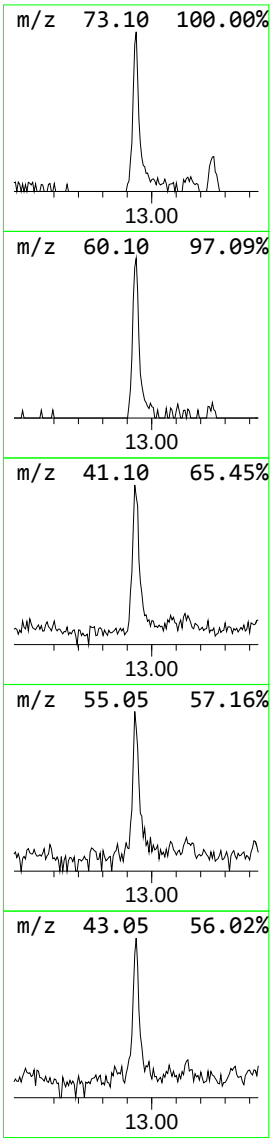
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanone, 1-(4,5-dihydro-2-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.936	5.26 ng	66585	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	50
2	1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	47
3	Alpha-l-rhamnopyranose	164	C6H12O5	035810-56-1	47
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	47
5	Hexanoic acid	116	C6H12O2	000142-62-1	43





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Acq On : 20 Jul 2022 17:22
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Sample : N3767-07 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-P

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

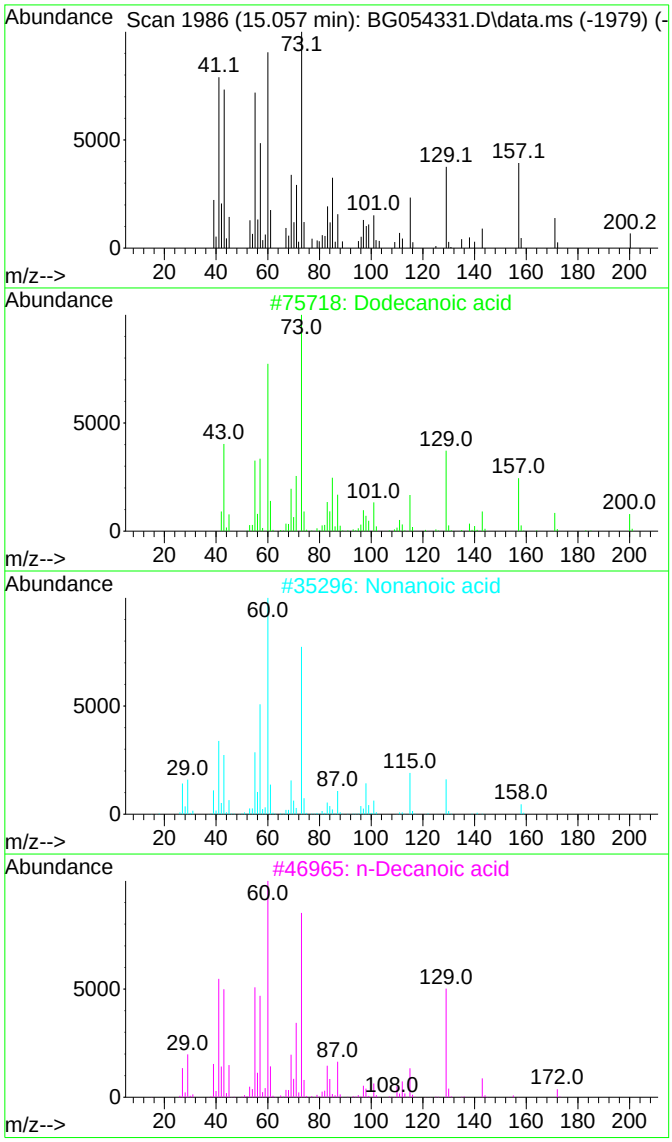
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

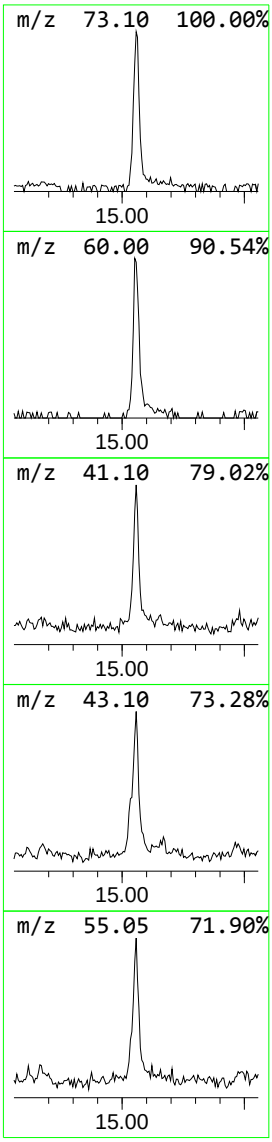
****

Peak Number 3 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	7.97 ng	100895	Acenaphthene-d10	14.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	97
2	Nonanoic acid	158	C9H18O2	000112-05-0	49
3	n-Decanoic acid	172	C10H20O2	000334-48-5	49
4	Undecanoic acid	186	C11H22O2	000112-37-8	47
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-P

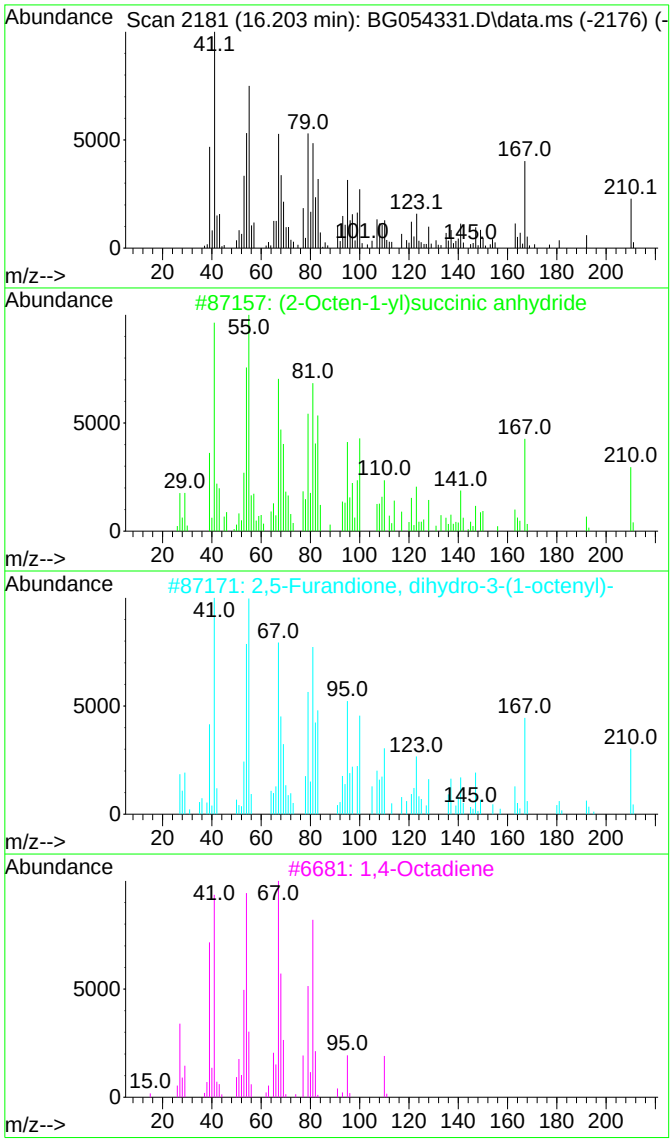
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

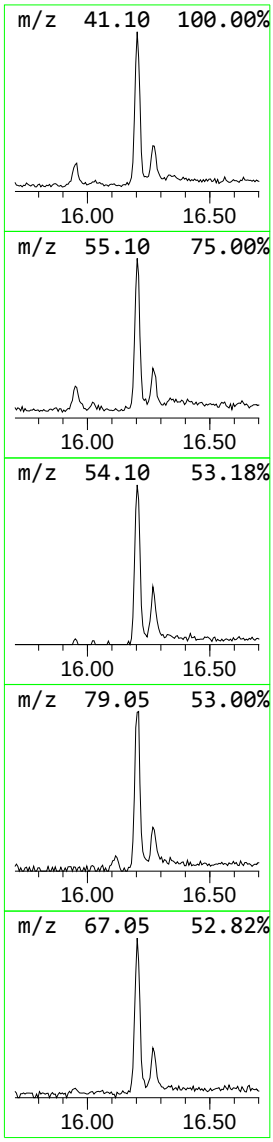
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (2-Octen-1-yl)succinic anhy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.203	11.73 ng	262736	Phenanthrene-d10	17.372

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2-Octen-1-yl)succinic anhydride	210	C12H18O3	042482-06-4	99
2	2,5-Furandione, dihydro-3-(1-oct...	210	C12H18O3	007757-96-2	94
3	1,4-Octadiene	110	C8H14	005675-25-2	83
4	trans-(2-Octenyl)succinic anhydride	210	C12H18O3	081949-84-0	60
5	Cyclooctene, 4-ethenyl-	136	C10H16	001124-45-4	46





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Data File : BG054331.D
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Sample : N3767-07 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
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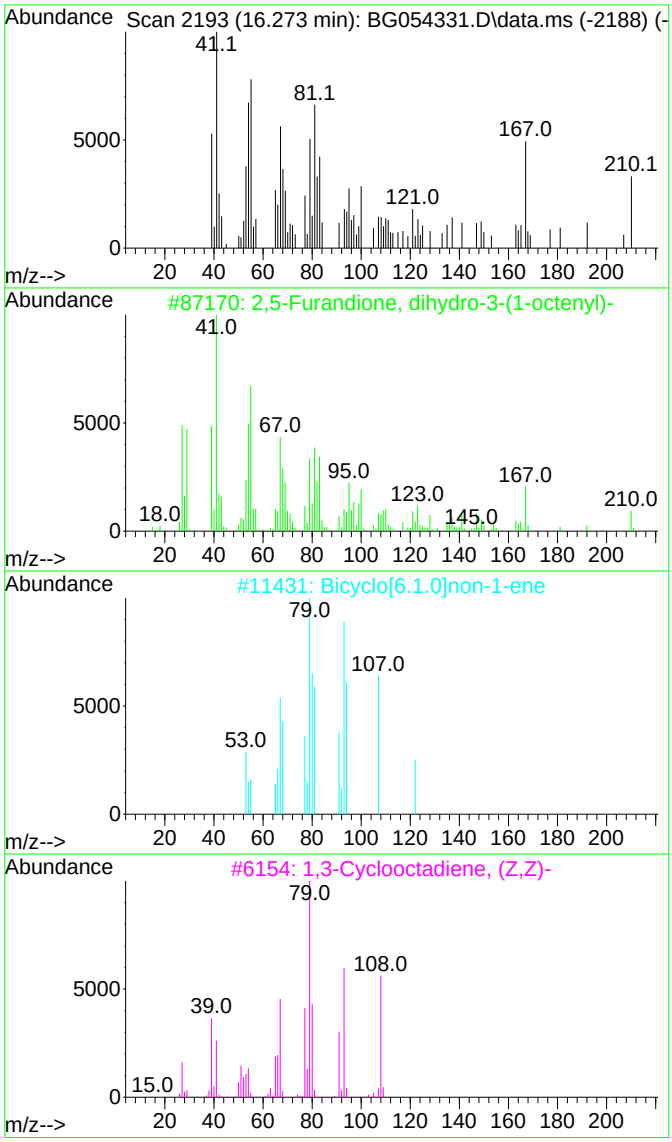
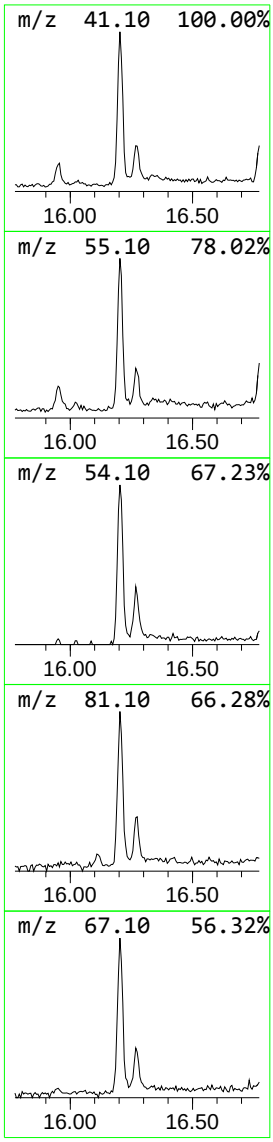
Peak Number 5 unknown16.273 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.273	2.83 ng	63516	Phenanthrene-d10	17.372

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Furandione, dihydro-3-(1-oct...	210	C12H18O3	007757-96-2	49
2	Bicyclo[6.1.0]non-1-ene	122	C9H14	002570-06-1	46
3	1,3-Cyclooctadiene, (Z,Z)-	108	C8H12	003806-59-5	45
4	1,5-Cyclooctadiene, (E,E)-	108	C8H12	017612-50-9	43
5	1,5-Cyclooctadiene, (E,Z)-	108	C8H12	005259-71-2	38





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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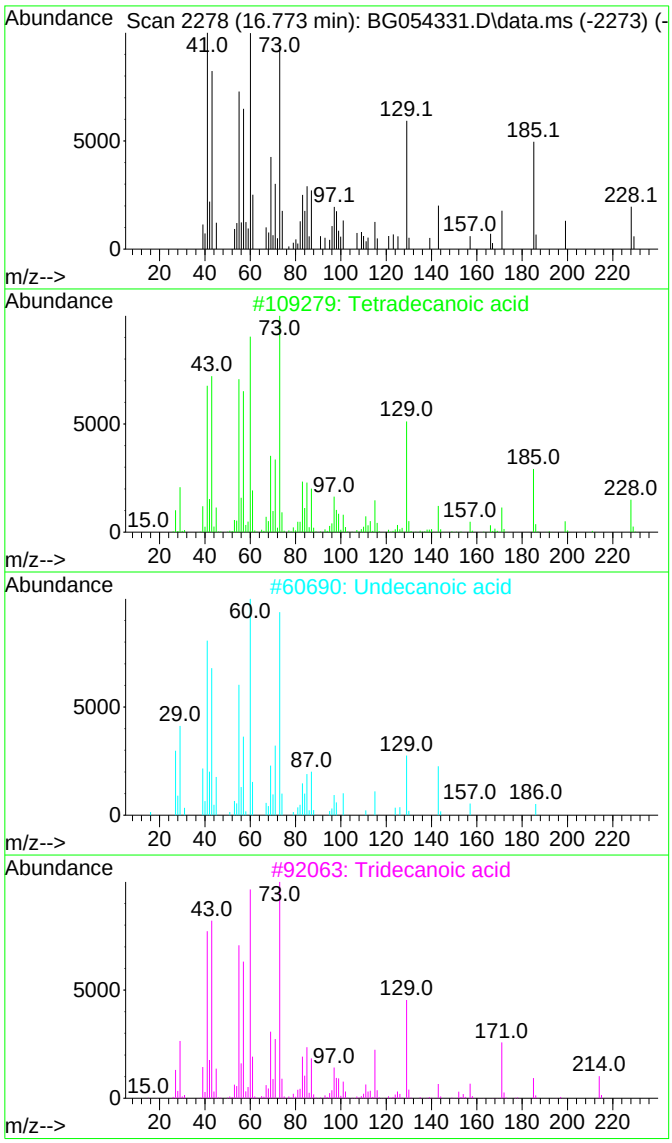
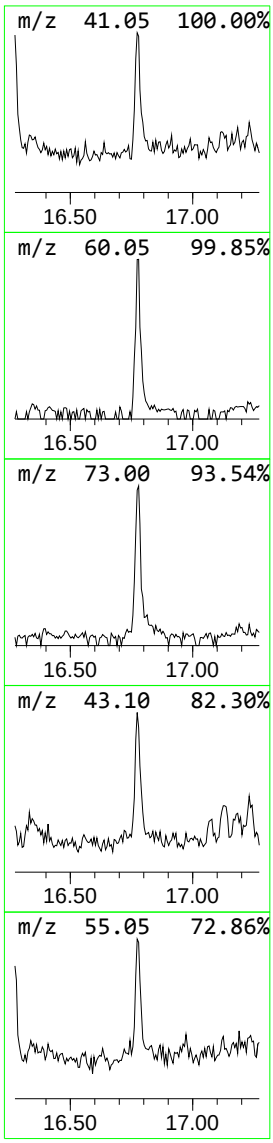
Peak Number 6 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.773	3.06 ng	68464	Phenanthrene-d10	17.372

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
2	Undecanoic acid	186	C11H22O2	000112-37-8	55
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-P

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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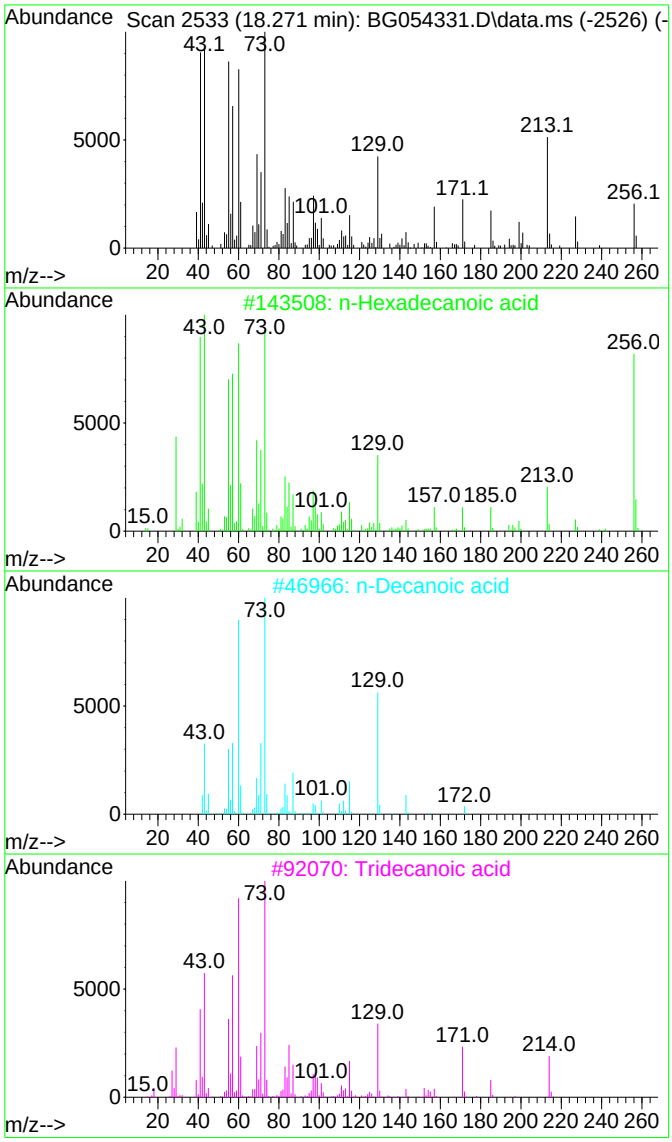
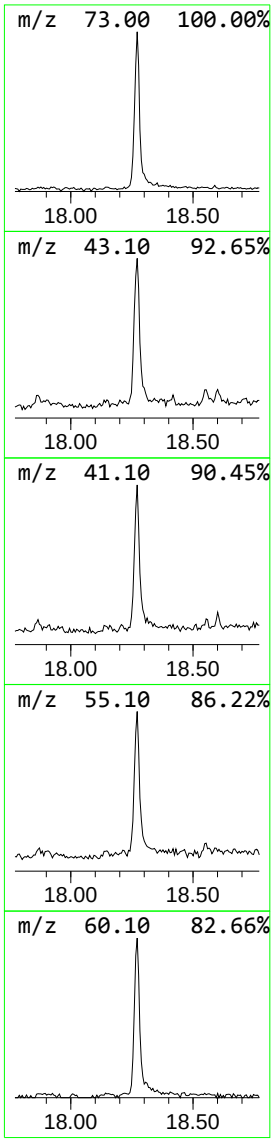
Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.271	13.61 ng	305016	Phenanthrene-d10	17.372

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





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TIC Library : C:\Database\NIST20.L
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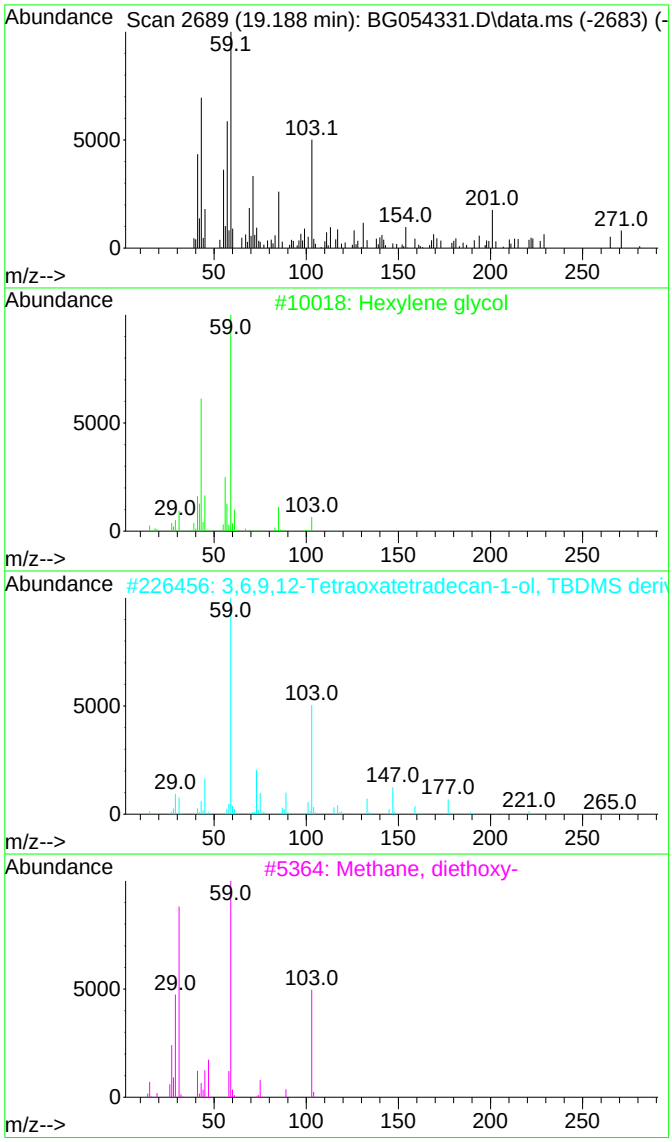
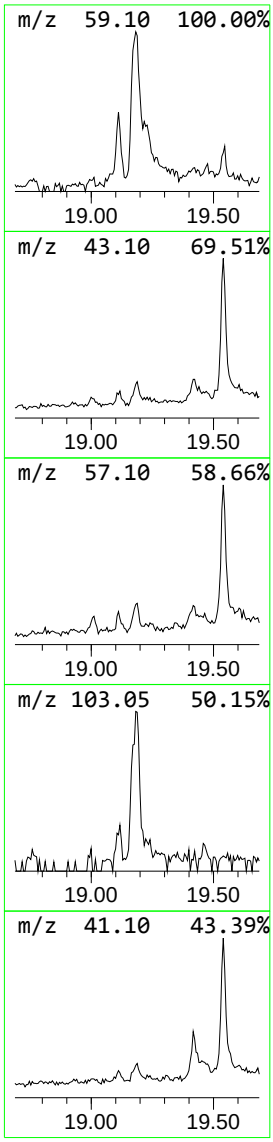
Peak Number 8 Hexylene glycol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.188	3.31 ng	74182	Phenanthrene-d10	17.372

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	50
2	3,6,9,12-Tetraoxatetradecan-1-ol...	322	C15H34O5Si	1000352-09-6	50
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	50
4	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	50
5	2-(2-methoxyethoxy)propanoic aci...	190	C8H14O5	1000506-61-7	40





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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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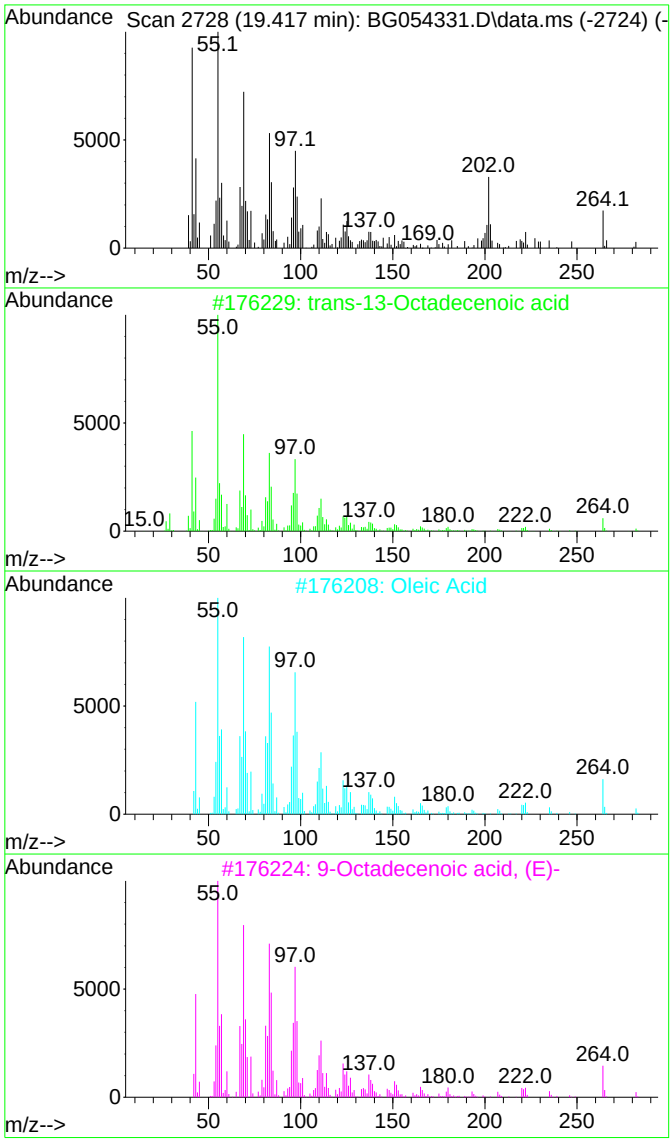
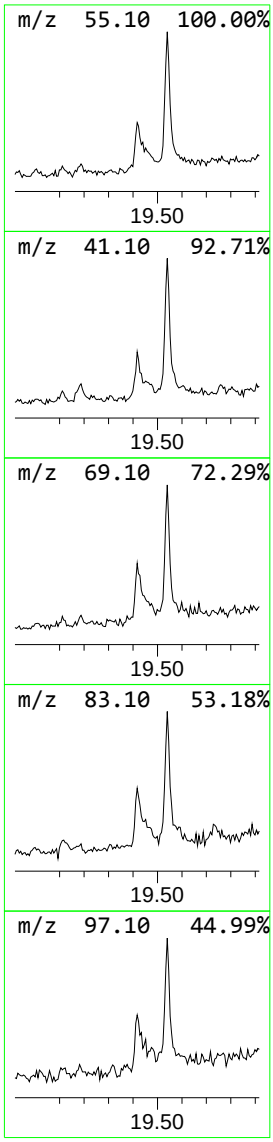
Peak Number 9 trans-13-Octadecenoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.417	6.61 ng	148198	Phenanthrene-d10	17.372

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	93
2	Oleic Acid	282	C18H34O2	000112-80-1	91
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	91
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	90
5	1-Dodecanethiol	202	C12H26S	000112-55-0	87





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Data File : BG054331.D
Acq On : 20 Jul 2022 17:22
Operator : CG/JU
Sample : N3767-07 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-P

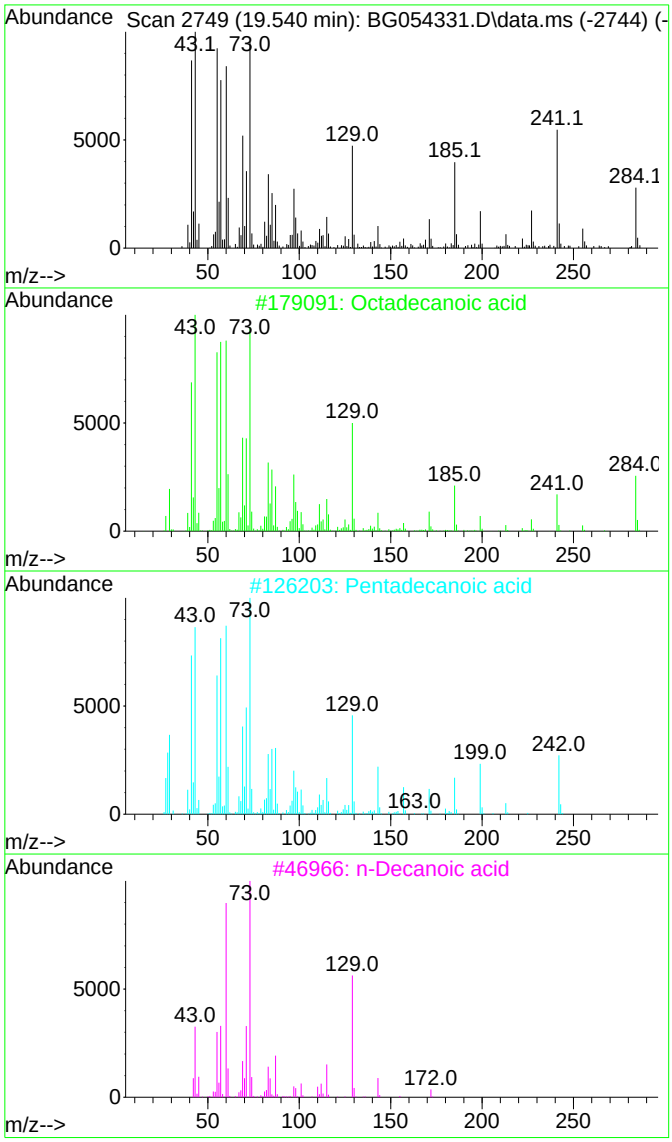
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

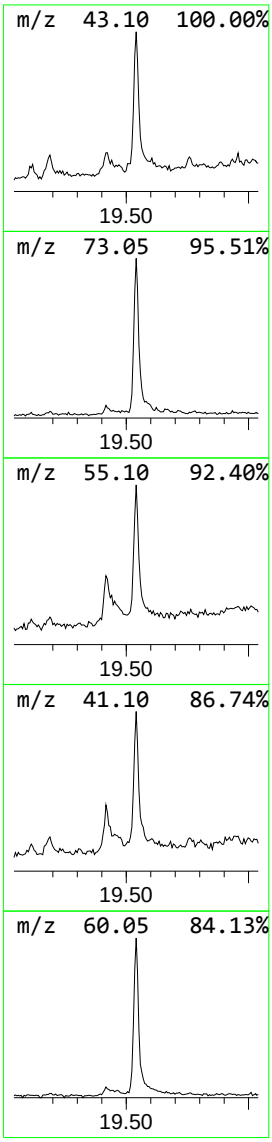
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.540	17.05 ng	358024	Chrysene-d12	21.644

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62





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Data File : BG054331.D
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Operator : CG/JU
Sample : N3767-07 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-P

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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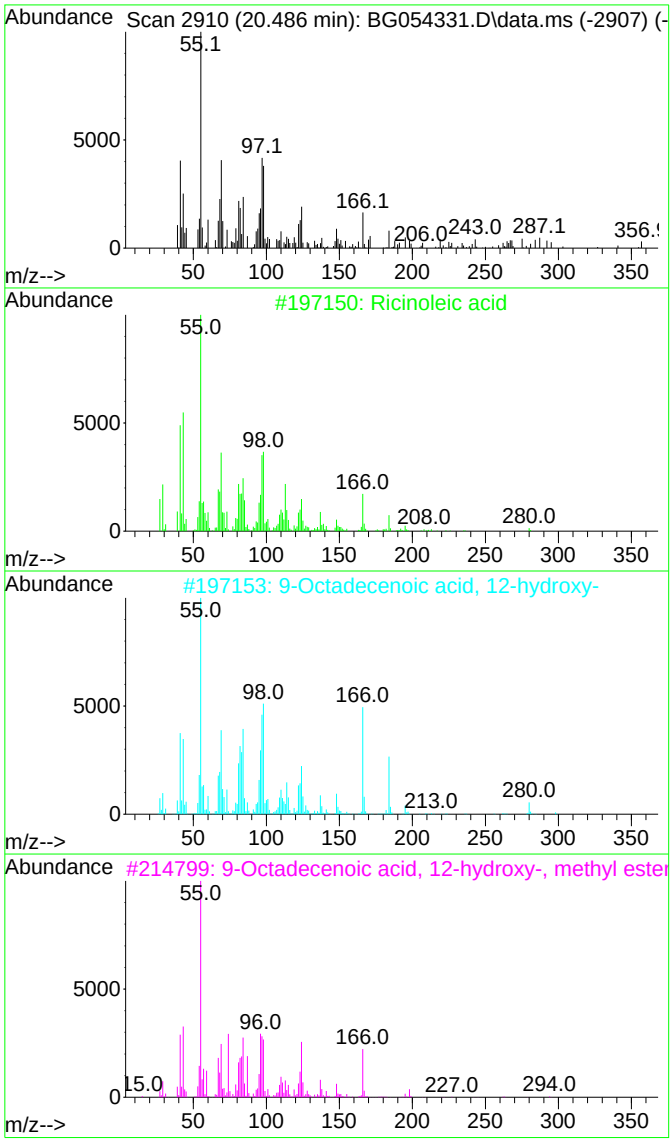
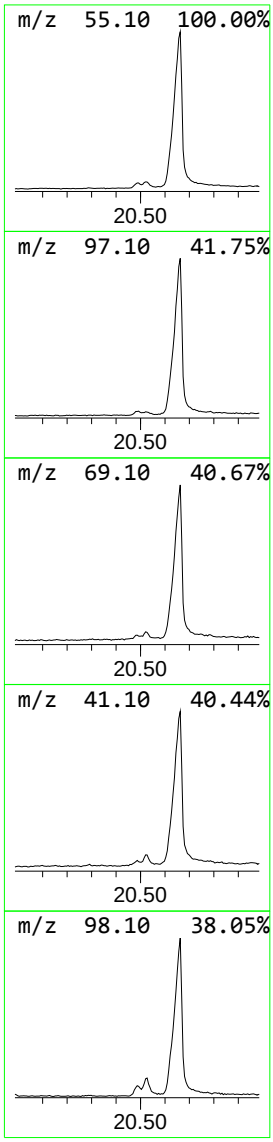
Peak Number 11 Ricinoleic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.486	3.15 ng	66168	Chrysene-d12	21.644

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ricinoleic acid	298	C18H34O3	000141-22-0	72
2	9-Octadecenoic acid, 12-hydroxy-	298	C18H34O3	007431-95-0	52
3	9-Octadecenoic acid, 12-hydroxy-...	312	C19H36O3	000141-24-2	27
4	Heptadecanolide	268	C17H32O2	005637-97-8	14
5	1-Cyclopenten-3-one, 1-(ethoxyca...	170	C8H10O4	1010164-70-4	14





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Data File : BG054331.D
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Operator : CG/JU
Sample : N3767-07 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-P

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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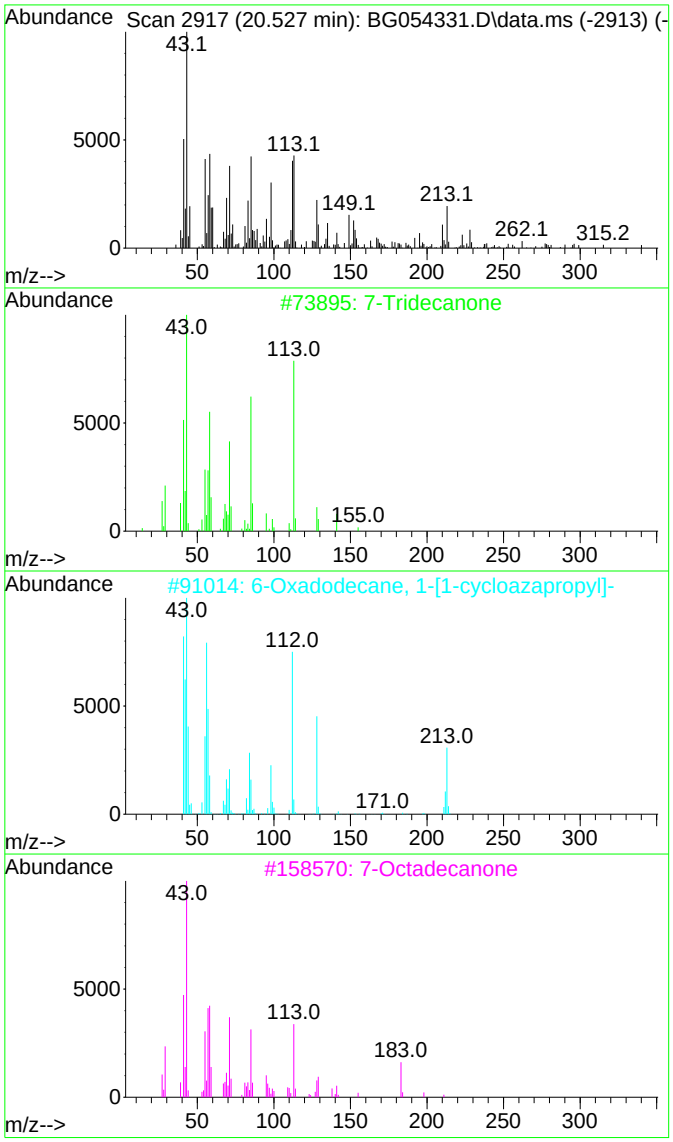
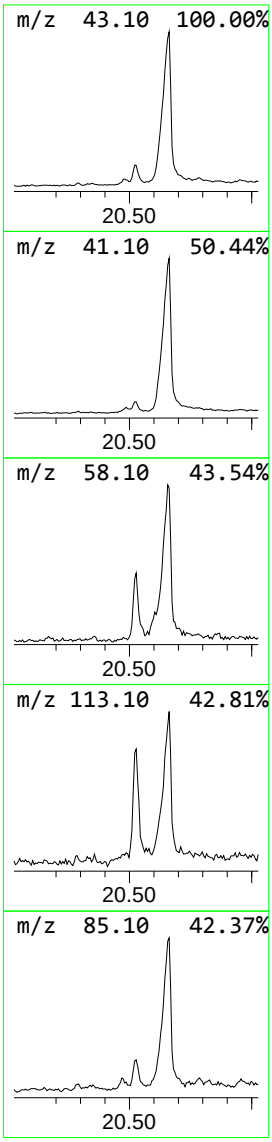
Peak Number 12 unknown20.527 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.527	9.63 ng	202243	Chrysene-d12	21.644

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Tridecanone	198	C13H26O	000462-18-0	32
2	6-Oxadodecane, 1-[1-cycloazaprop...	213	C13H27NO	1000251-59-0	27
3	7-Octadecanone	268	C18H36O	018277-00-4	22
4	7-Heptadecanone	254	C17H34O	006064-42-2	22
5	3-Nonanone	142	C9H18O	000925-78-0	18





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Operator : CG/JU
Sample : N3767-07 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-P

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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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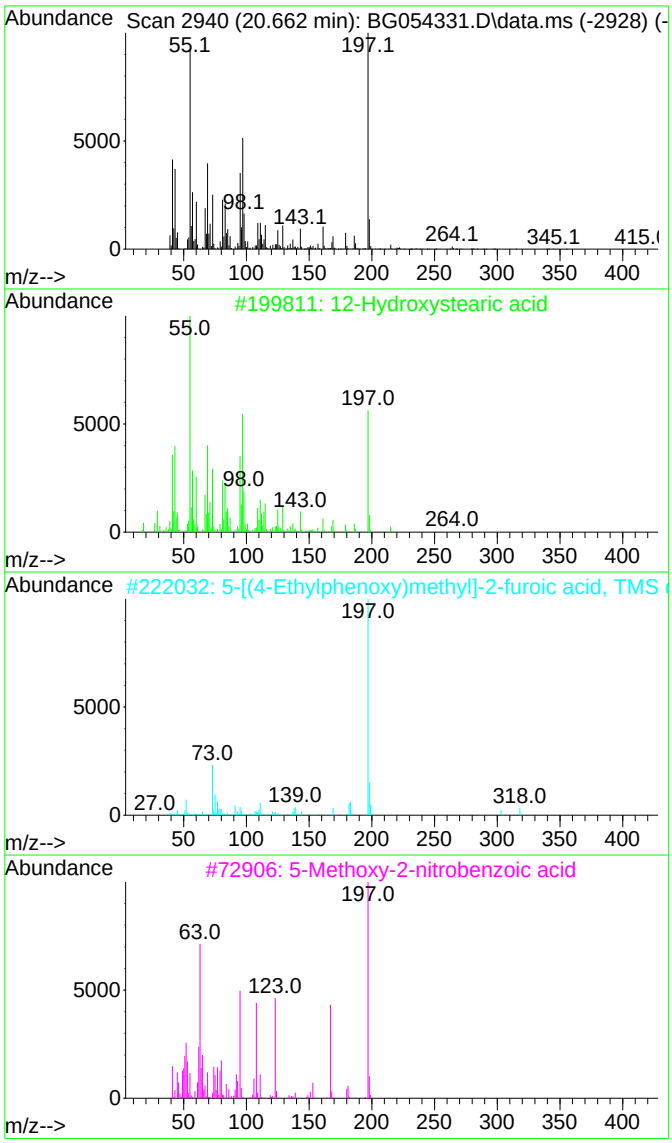
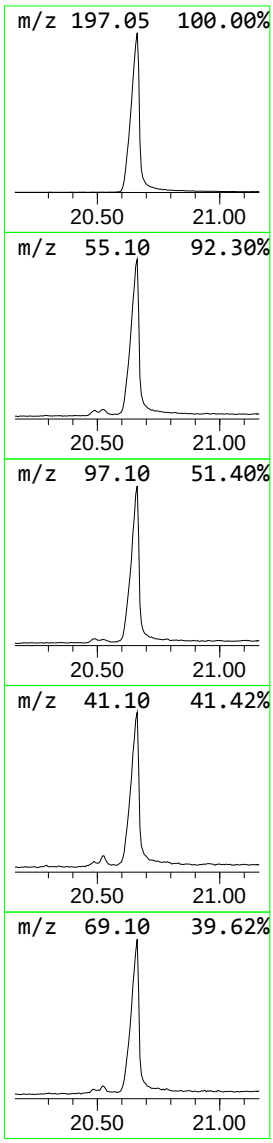
Peak Number 13 12-Hydroxystearic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.662	286.65 ng	6020670	Chrysene-d12	21.644

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	76
2	5-[(4-Ethylphenoxy)methyl]-2-fur...	318	C17H22O4Si	1000474-93-6	38
3	5-Methoxy-2-nitrobenzoic acid	197	C8H7NO5	001882-69-5	35
4	p,p'-Ditolylamine	197	C14H15N	000620-93-9	30
5	2-(4-Cyanophenyl)-5-hydroxypyrim...	197	C11H7N3O	150405-59-7	30





Tentatively Identified Compound (LSC) summary

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Data File : BG054331.D
Acq On : 20 Jul 2022 17:22
Operator : CG/JU
Sample : N3767-07 5X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-P

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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
Nonanoic acid	11.638	10.0	ng	75396	2	10.803	150161	20.0
Ethanone, 1-(4,...	12.936	5.3	ng	66585	3	14.628	253176	20.0
Dodecanoic acid	15.057	8.0	ng	100895	3	14.628	253176	20.0
(2-Octen-1-yl)s...	16.203	11.7	ng	262736	4	17.372	448102	20.0
unknown16.273	16.273	2.8	ng	63516	4	17.372	448102	20.0
Tetradecanoic acid	16.773	3.1	ng	68464	4	17.372	448102	20.0
n-Hexadecanoic ...	18.271	13.6	ng	305016	4	17.372	448102	20.0
Hexylene glycol	19.188	3.3	ng	74182	4	17.372	448102	20.0
trans-13-Octade...	19.417	6.6	ng	148198	4	17.372	448102	20.0
Octadecanoic acid	19.540	17.1	ng	358024	5	21.644	420074	20.0
Ricinoleic acid	20.486	3.1	ng	66168	5	21.644	420074	20.0
unknown20.527	20.527	9.6	ng	202243	5	21.644	420074	20.0
12-Hydroxystear...	20.662	286.6	ng	6020670	5	21.644	420074	20.0